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THEROETICAL TRAJECTORIES OF CHARGED PARTICLES IN AN INHOMOGENEOUS MAGNETIC FIELD

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THEORETICAL TRAJECTORIES OF CHARGED PARTICLES IN AN INHOMOGENEOUS MAGNETIC FIELD

by

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ABSTRACT

This theoretical study of the trajectories of charged particles supplements an experimental project of molecular-ionic rearrangements using the magnetic focusing properties of a beta-ray spectrometer. The experimentally measured magnetic field was analytically represented by a twelfth-order polynomial. This field is axially symmetric, but non-homogeneous otherwise. The particular particle of concern was the hydrogen ion, H_2^+. The trajectory of this particle was computed from a second-order differential equation, assuming values for the kinetic energy and initial angle of the particle, and the magnetizing current. The solution was obtained by numerical integration using a CDC 1604 digital computer. The distinctive feature of these calculations, in contrast to those used normally for a beta-ray spectrometer, is the large scattering (initial) angle, about 45°.

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TABLE OF SYMBOLS

A	The vector potential
B	The magnetic flux density of the field
B(i)	The coefficients computed for the polynomial which describes the magnetic field on-axis
E	The kinetic energy of the rebound particle, a function of the scattering angle
E_o	The energy of the incident particle
Fi, Gi	Functions of z which are described later in detail
$H_o(z)$	The axial component of the field on axis
H^i	The i-th derivative of the function $H_o(z)$
I_B	The magnetization current
$k = p/q$	
L	The intercept distance measured on the z-axis
ϕ	The azimuthal angle in cylindrical coordinates
p	The momentum of the rebound particle (H_2^+)
q	The magnitude of the electronic charge
r	The radial distance in cylindrical coordinates
θ	The scattering angle measured in the laboratory frame
z	The axial distance in cylindrical coordinates

1. Introduction

This presentation is part of an experimental project presently being conducted at the U. S. Naval Postgraduate School to verify a classical theory developed by Bates, Cook, and Smith [1] of the capture of a light ion or atom from a target system by a fast projectile.

Specifically, the theory involves a reaction of the type:

$$H^+ + CH_4 \rightarrow H^+H + CH_3$$

and is essentially a sequence of binary collisions. The process ensues with the bombardment of methane gas by low energy protons, whereby the resulting rebound proton and escaping hydrogen ion join to form the product H_2^+. The angle of departure (or scatter) is shown to be in the vicinity of 45 degrees, and is labeled θ.

Since the expected cross section will be quite low ($\leq 10^{-18}$ cm^2), a detector could not be utilized, as is standard procedure, by placement at the scattering angle. [5]

Therefore, the beta-ray spectrometer was chosen due to its property which will cause all H_2^+ ions of the same departure angle and energy to converge. This study determines that point of convergence, or focus.

2. Discussion

It is known from elementary electromegnetic theory that a magnetic force, $q\{\vec{v} \times \vec{B}\}$, is produced on a charged particle moving at an angle to the direction of the field. This force causes the particle to sustain a change in velocity (direction only). The supposition is, for this field, that a particle which begins its motion on the axis of the field and at an angle with that field axis, will travel a curvilinear path and ultimately intersect the axis of the field for appropriate values of the field strength, energy and initial angle of the particle. This can be readily shown for a homogeneous field.

The point at which the particle returns to the axis is called the intercept point, and the distance from the origin of the trajectory to the intercept point is the intercept distance (L). This is where the

detector can be placed to analyze the particulate beam. The experimental usefulness is that if the intercept distance is known along with the field strength, and the energy of beam E_o, then the initial angle may be evaluated.

The theoretical problem, which is herein shown, is the evaluation of the intercept distance assuming values for the scattering angle.

Thus, the following intermediate problems arose:

A. A means to express the field, or more precisely, a continuous function which would represent the field for all points in the area of interest.

B. A set of equations to specify the motion of the particle to incorporate the energy and charge of the particle, as well as the interaction of the magnetic field.

C. A numerical method to solve a differential equation which would result from the equations in (B) above.

D. Interpretation and extrapolation from sets of trajectories to obtain these derivatives:

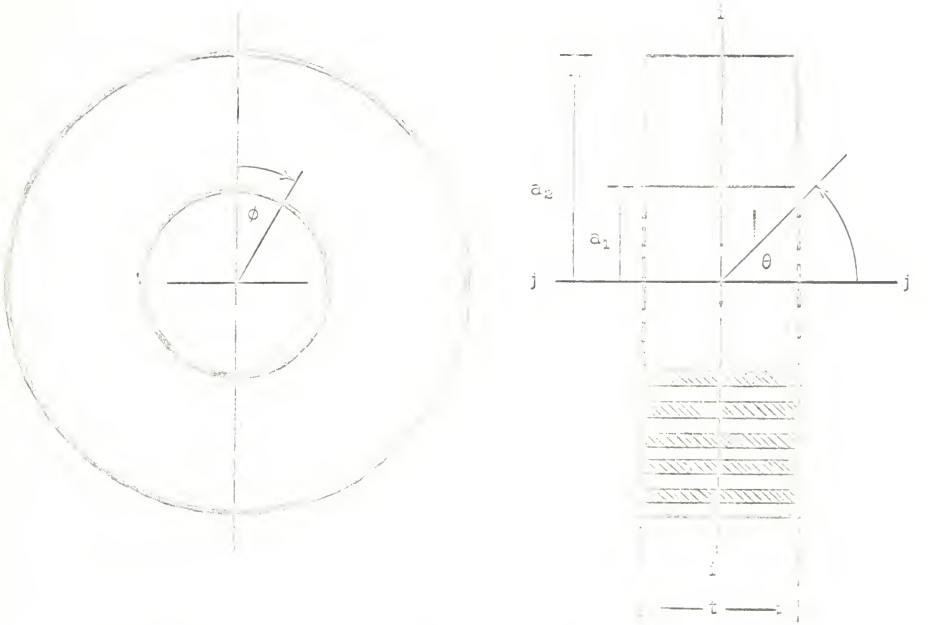
$\left(\frac{\partial L}{\partial E}\right)_{\theta,\ I_B}$ -- The change in intercept distance with respect to changes in energy

$\left(\frac{\partial L}{\partial \theta}\right)_{I_B,\ E_o}$ -- The change in intercept distance with respect to changes in angle

$\left(\frac{\partial L}{\partial I_B}\right)_{E_o,\ \theta}$ -- The change in intercept distance with respect to changes in magnetization current

3. The Magnet and its Field

The magnet which will be used for this project was previously in the USNPGS beta-ray spectrometer. It is essentially composed of a normal section of a right circular cylinder, and wound with cylindrically concentric layers of copper wire. The outer disks and cylindrical center section which form the container for the layers of wire are copper as are the cooling water tubes. The figure (Fig. 1) on the next page shows the magnet with its dimensions.



Blank layers indicate water cooling tubes
Cross-hatched layers, copper wire

a_1 = Inside radius of the coil = 10.17 cm.

a_2 = Outside radius of the coil = 27.30 cm.

t = Thickness of the coil = 15.78 cm.

Fig. 1. The Magnet

The experimental field strength of this magnet on-axis, H_o, appears as a Gaussian curve as shown in Fig. 2. The quantities in Appendix 1 for the values of the field are shown in the positive z direction. The maximum intensity of the field on-axis is at the geometrical center of the magnet, at the point formed by the intersection of lines ii and jj. B has cylindrical symmetry about the line jj, and is symmetrical about the center plane.

In order to more easily discuss the field, the system of cylindrical coordinates should be established at this point. The origin is defined to be at the intersection of the lines ii and jj. The line jj will be the z axis, and the radial distance, r, will be measured perpendicularly from it. The angular component, ϕ, is as in (r, ϕ, z), a right hand coordinate system.

Measurements were made on this field for various values of field current by P. J. Kelly in May 1965 with an axial Hall Probe, and this data has been compiled in Appendix 1. The axial component of the field intensity was measured initially on the primary axis of the magnet (z axis) for a distance of 66 cm. on either side of the origin at 4 cm. intervals. This was done for various current settings between 2 and 14 amperes.

Also, the axial component of the field was measured off axis at four values of z, and for 8 values of ϕ, for each value of z. The radius r was varied from zero to seven cm.

The conclusions concerning the field were that:

(1) The field strength is linear with current over the entire range of current settings within an accuracy of ±0.1%.

(2) The field is symmetrical on either side of the $z = 0$ plane to ±0.01%.

(3) The field is azimuthally symmetric to ±0.01%.

To find the analytic expression for the field on axis, $H_o(z)$, where z assumes positive values only, a polynomial was fit to the data by the method of least-squares. This data is contained in Appendix 1. A

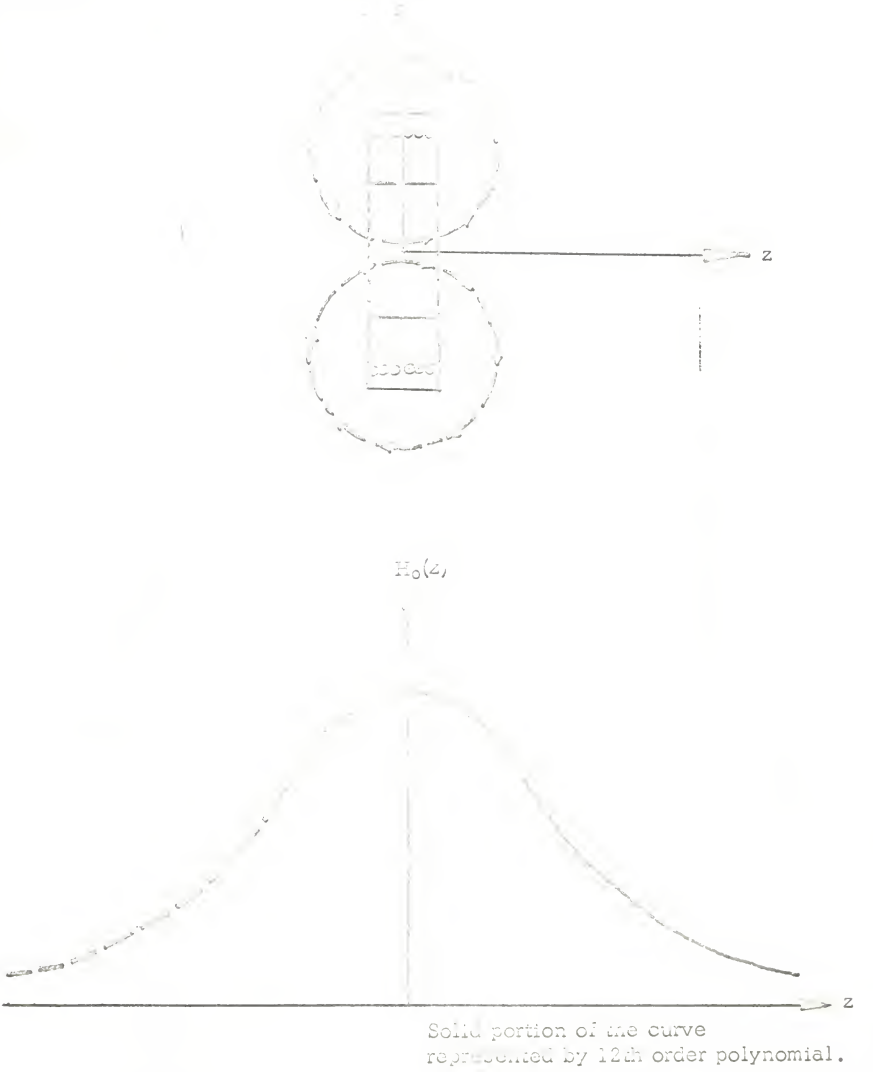


Fig. 2. The Magnetic Field

twelfth order polynomial was chosen, and provided sufficient precision in the form:

$$H_o(z) = B_1 + B_2 z + B_3 z^2 + B_4 z^3 + B_5 z^4 + \ldots + B_{13} z^{12} \quad . \qquad (3\text{-}1)$$

The thirteen coefficients were determined by the computer and a USNPGS subroutine LSQPOL, which is in PROGRAM CURVE included in Appendix 6.

At this point, a comparison was made of the experimental field values and those values which would result from the polynomial field expression.

To make this check of the values of the field off-axis, the following steps were taken:

(1) The vector potential was computed for all values of r and z using the derived polynomial.

(2) The axial component of the field was derived, using the vector potential, and evaluated for various values of r and z.

This computation is shown in detail in Appendix 1. The agreement between experimental and theoretical values was again quite good.

4. Theory of the Trajectory

The H_2^+ ion has a positive charge equal in magnitude to that of the electron, and mass essentially equal to twice the mass of a single proton. The mass of the single electron is ignored.

The path of this particle can be represented by this equation:

$$\left[\frac{r''}{1 + (r')^2}\right] \{k^2 - A^2\} - r'(A) \left[\frac{\partial A}{\partial z}\right] + A \left[\frac{\partial A}{\partial r}\right] = 0 \qquad (4\text{-}1)$$

where A is the vector potential, and k is defined as (mv/q). The prime above indicate differentiation with respect to z. A discussion of A, its derivatives, and k will follow.

This equation for any charged particle can be derived from the equations of motion for that particle which begins its path on the primary axis of the magnetic field. This equation is derived in Appendix 4.

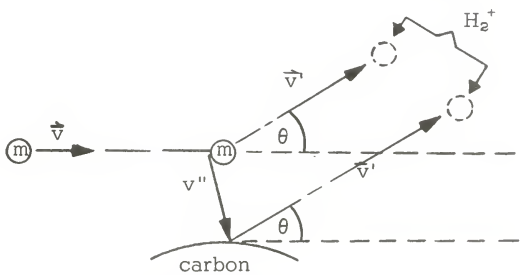
The energy of the H_2^+ particle after scattering is E, and can be shown to be:

$$E = 2\ E_o\ \cos^2\ \theta \qquad (4\text{-}2)$$

where E_o is the kinetic energy of the particle which is incident on the target methane. The angle θ is again the angle of scatter.

A description of the collision process is as follows:
The incoming proton strikes one of the hydrogens in the methane molecule. This is the first of the two binary collisions, and the only one which is assumed to be totally elastic. The initial particle moves off at an angle, called the departure angle; and the second particle (essentially a proton and an electron) moves towards the carbon atom at an angle equal to $90^o - \theta$. Since the carbon atom is assumed to be infinitely massive, compared to the hydrogen atom approaching it, this second particle is redirected in the second binary collision in the direction of the recoiling proton.

A schematic of the collision process is as follows:



In the laboratory frame, the initial energy of the system is:

$$E_o = \tfrac{1}{2}\, m_1\ (\vec{v}_1)^2 \qquad (4\text{-}3)$$

and the final energy is:

$$E = \tfrac{1}{2}\,(2m)(\vec{v}')^2 \qquad (4\text{-}4)$$

Conservation of momentum yields, for the first collision:

$$P_x\ = m\vec{v}\ =\ m\vec{v}'\ \cos\ \theta\ +\ m\vec{v}''\ \sin\ \theta \qquad (4\text{-}5)$$

and,

$$p_y = m\vec{v}' \sin\theta - m\vec{v}'' \cos\theta = 0 \tag{4-6}$$

The last equation results in

$$\vec{v}'' = \vec{v}' \tan\theta \tag{4-7}$$

and substituting into the equation (4-5)

$$\vec{v}' = \vec{v} \cos\theta \,. \tag{4-8}$$

With this relationship between the velocities, the final energy after the two collisions becomes

$$E = \tfrac{1}{2}(2m)\,(\vec{v}')^2 \tag{4-4}$$

$$= \tfrac{1}{2}(2m)\, v^2 \cos^2\theta$$

$$= 2E_o \cos^2\theta$$

$$E = 2E_o \cos^2\theta \tag{4-2}$$

If both collisions are elastic in nature, then it is quite easy to show that θ must be 45°. The y-component of momentum produces the equation

$$p_y = m\vec{v}' \sin\theta - m\vec{v}' \cos\theta = 0 \tag{4-9}$$

at the first collision. And it can only be satisfied when

$$\sin\theta = \cos\theta$$

or, when $\theta = 45^\circ$.

5. Expression for the Vector Potential

The fact that the field is cylindrically symmetric carries with it the implication that there is no azimuthal component, since the curl B = zero. This field can be described by a vector potential which is always in the azimuthal direction.

Using the calculated expression for magnetic field on-axis, $H_o(z)$, the vector potential expansion

$$A(r,z) = \frac{r}{2} H_o(z) - \frac{r^3}{16}\left(\frac{\partial}{\partial z}\right)^2 H_o(z) + \frac{r^5}{384}\left(\frac{\partial}{\partial z}\right)^4 H_o(z) \tag{5-1}$$

$$+ \ldots + \frac{(-1)^n}{n!\,(n+1)!}\left(\frac{r}{2}\right)^{2n+1}\left(\frac{\partial}{\partial z}\right)^{2n} H_o(z) + \ldots$$

is shown to be for any point (r,z):

$$A = \frac{r}{2}[G_1] - \frac{r^3}{16}[G_2] + \frac{r^5}{384}[G_3] - \frac{r^7}{18432}[G_4] + \frac{r^9}{1474560}[G_5]$$

$$- \frac{r^{11}}{176947200}[G_6] + \frac{r^{13}}{29727129600}[G_7]$$

where $\left(\frac{\partial}{\partial z}\right)^n H_0(z)$ is the nth partial derivative of the function $H_0(z)$ with respect to z, and where $G_1 = H_0(z)$, and $G_2 = \left(\frac{\partial}{\partial z}\right)^2 H_0(z)$, etc.

6. The Computer Solution

It remains, at this point, to find the solution of the differential equation. The method chosen for this task was a process of numerical integration employing a digital computer. The subroutine INTEG-1 of the USNPGS Computer Library was selected because of its adaptability to this particular problem. The program in which INTEG-1 is contained is called PROGRAM ORBITS, and is listed as Program C in Appendix 6.

The first four statements of this program (ORBITS) are standard according to the instructions for use of INTEG-1. The three comment cards that follow describe ENER, OKAY, and P, which are names given various quantities used in the solution.

B(1) through B(13) are the coefficients used in the polynomial as obtained by PROGRAM CURVE. The functions F(1) through F(6), and G(1) through G(7) are explained in Appendix 5.

VECDZ is the symbol for the partial derivative of the vector potential with respect to z. VECDR represents the partial derivative of the vector potential with respect to r. VECPT is the vector potential.

A second order differential equation can be reduced to a system of two first differential equations. Applying this technique to equation (4-1) yields

$$[r']' = r' \frac{\left[A \frac{\partial A}{\partial z}\right]}{[k^2 - A^2]} + (r')^3 \frac{\left[A \frac{\partial A}{\partial z}\right]}{[k^2 - A^2]} - (r')^2 \frac{\left[A \frac{\partial A}{\partial r}\right]}{[k^2 - A^2]} - \frac{\left[A \frac{\partial A}{\partial r}\right]}{[k^2 - A^2]} \qquad (6\text{-}1)$$

$$[r]'' = r' \qquad (6\text{-}2)$$

Letting

$$x(1) \equiv r \qquad \text{and} \quad x(2) \equiv r' ,$$

the equations (6-1) and (6-2) become

$$[x(2)]' = [x(2)]\,FUNC4 + [x(2)]^3\,FUNC4 - [x(2)]^2\,FUNC5 - FUNC5$$

$$[x(1)]' = x(2)$$

where

$$FUNC4 = \frac{[A\ \frac{\partial A}{\partial z}\ ]}{[k^2 - A^2\ ]}$$

$$FUNC5 = \frac{[A\ \frac{\partial A}{\partial r}\ ].}{[k^2 - A^2\ ]}$$

Further, FUNC4 and FUNC5 can be written in terms of FUNC1, FUNC2 and FUNC3 as follows:

$$FUNC1 = k^2 - A^2$$

$$FUNC2 = A\,\frac{\partial A}{\partial z}$$

$$FUNC3 = A\,\frac{\partial A}{\partial r}$$

and

$$FUNC4 = \frac{FUNC2}{FUNC1}$$

$$FUNC5 = \frac{FUNC3}{FUNC1}$$

OKAY is obtained in the following way. This is the machine language expression for k^2 where the energy can be entered in eV. In the MKS system, k must have the unit of webers/meter. This is the same as A, since B has the units of webers/meter^2, and $\vec{B} = \vec{\nabla} \times \vec{A}$.

$$k = \frac{m\,v}{q} \quad \text{in units of} \quad \frac{(\text{kilogram})(\text{meter/sec})}{(\text{coulombs})} \quad \text{or webers/meter.}$$

It would be desirable to have k expressed in terms of the energy of the particle, E, and in the units of eV, as a great savings in conversion would be realized.

Using the non-relativistic expression for the energy E, the following is obtained:

$$E = \frac{p^2}{2m} \qquad \therefore\ p = (2mE)^{\frac{1}{2}}$$

But, since k^2 is needed

$$k^2 = \frac{p^2}{q^2} = \frac{2mE}{q^2} = \frac{2mE'}{q} \qquad \text{if } E' \text{ is expressed in eV.}$$

And, k^2 becomes

$$\left[\frac{2(\text{mass of } H_2^+)}{\text{charge of electron}}\right] E'$$

Inserting the values of the constants, k^2 becomes the quantity OKAY:

$$OKAY = \left\{\frac{4(1.6725 \times 10^{-27}}{1.6021 \times 10^{-19}}\right\} E'$$

$$= \{4.17576 \times 10^{-8}\} E'$$

or

OKAY = (4.17576E - 08)*(ENER), as expressed in the program.

The method of solution employed by INTEG-1 is a fourth order Runge-Kutta numerical integration approximation of the ordinary differential equations.

The computation is performed in the MKS system of units.

TO USE PROGRAM ORBITS (the main trajectory program)

This program is written in the language of FORTRAN-60. Its successful employment depends on the correct use of the data cards, which are the last eight cards of the program itself. These eight cards contain the input information, and the quantities desired as output. An example of the data cards may be seen on the last page of Program C in Appendix 6.

Data card #1: This card is used for identification, and columns 2-32 are available for this use. This title appears on all data output, as well as graphs.

Data card #2: This card contains the number of "runs", or trajectories, to be processed with a maximum of 9. This number is entered in column 1 of the card. Note, however, that only one graph is possible for the entire program.

Data card #3: The number of coupled first-order differential equations is specified by this card (maximum of 30). In this case, there are two and this number is posted, right justified, in columns 1 and 2, as 02.

Data card #4: The initial and final values of the independent variable, z, over which the integration process is to be carried out. The integration step size is also stipulated. The integration can be processed in up to 3 segments, each with a different step size, thus:

$$ZI \xrightarrow{S1} Z1 \xrightarrow{S2} Z2 \xrightarrow{S3} ZF,$$

or $ZI \xrightarrow{S1} Z1 \xrightarrow{S2} ZF$,

or $ZI \xrightarrow{S1} ZF$,

where ZI refers to the initial value of z (in this case equal to zero), ZF refers to the final value of z, Zi refers to intermediate values of z, and Si are the step sizes. All of these numbers are entered in meters. The corresponding values, with decimal points, are placed in the above order in columns 1-10, 11-20, 21-30, etc.

Data card #5: Columns 1-10 contain the value of the energy E in electron-volts, again, with the decimal point. Columns 11-20 contain the quantity P which adjusts the magnetic field according to

the base of 10 amperes magnetization current. For example, for a field of 7 amps, the quantity 0.70 would be entered anywhere in columns 11-20.

Data card #6: Here are the values of the initial conditions. The format is the same as for cards 4 and 5. The first value expressed is the initial value of r (equal to zero), and the next value is the slope of the function at that point, $\left(\frac{dr}{dz}\right)$. This derivative may be considered to be also the tangent of the scattering angle, θ.

Data card #7: This card controls data print-out. A blank card will suppress this output. Again, using the ten column sequence, this format is as follows. The first 8 columns contain the title for each variable output desired, and the last two columns contain the variable identifier. The variable identifiers are 00 for z, 01 for r, and 02 for r'. An example: Z DIST 00R DIST 01SLOPE 02

Data card #8: This last data card controls graph output. A blank card will suppress this output. Remember: that only ONE graph for each submitted program can be drawn and it corresponds to the first set of data. The information is contained in columns 1-20. Columns 1-16 contain the graph title, and columns 17-20 indicate the variable identifiers. Columns 17-20 must always be 0100. The origin, direction of plot, and scale distances have already been set within the main program.

Running Time: The time required for the computer solution is dependent on the step size and the total range of the independent variable. This running time has averaged about three minutes for a single trajectory.

7. Results

The outcome of this project was the creation of a single-package system which generates hydrogen ion trajectories in an axially symmetric field.

Approximately 100 production trajectories were computed for values of energy E ranging from 97 eV to 450 eV; magnetizing current from 7 to 15 amperes; and scattering angle of 35-55 degrees. The

numerical output data and the graph plots showed these orbit configurations to be quite smoothly continuous and consistent.

The error in evaluating the intercept distance L was due mainly in the uncertainty of reading the graph or interpolating the data printout. These values of L ranged from 20 centimeters to about 80 centimeters, with an estimated error of ±1.0%. The maximum radial distance of the orbits was around 8 cm.

Comparison of these computer trajectories with those obtained by the fine wire technique used by Kelly showed only fair agreement to within ±10.0%. The disparities in the different sets of trajectories have not as yet been determined.

This computer system was checked with a constant uniform (homogeneous) magnetic field against an analytic solution. The comparative results were excellent (to within ±0.01%).

Based on a Standard Trajectory of E_o = 300 eV,

I_B = Magnet current = 12 amperes,

θ = 45 degrees:

$$\left(\frac{\partial L}{\partial \theta}\right)_{E_o,\, I_B} = -3.3 \pm 0.2 \text{ cm/deg}$$

$$\left(\frac{\partial L}{\partial I_B}\right)_{\theta,\, E_o} = -9.7 \pm 0.8 \text{ cm/amp}$$

$$\left(\frac{\partial L}{\partial E_o}\right)_{I_B,\, \theta} = 0.20 \pm 0.01 \text{ cm/eV}$$

The above derivatives show that as θ and I_B are increased, L is decreased. However, an increase in E_o produces an increase in L. Each of the partial derivatives were obtained with respect to a change in a single parameter, with the other two parameters held constant.

8. Acknowledgements

In this limited space and manner, I note with pleasure all those people from whom I have received impetus towards the completion of this study. To them, I render my personal appreciation.

I wish to thank Professors F. D. Faulkner and H. M. Martinez of the Department of Mathematics, Professors F. W. Terman and J. R. Ward of the Electrical Engineering Department, and Professors O. Heinz and R. L. Armstead of the Physics Department for their inspiration, encouragement and assistance.

Prof. Ward provided invaluable assistance and advice as to the modification of the integration and draw systems of the main trajectory program. Prof. Heinz, at whose suggestion and under whose guidance the central project is being undertaken, contributed his ideas and enthusiasm. Prof. Armstead, as my thesis advisor, aided with his timely counsel, helpful suggestions and continued confidence; and to him, I am sincerely indebted.

To all the personnel of the Computer Facility, USNPGS, and, in particular, Mrs. Robin Ekstrum, I salute for their extreme consideration. Without their cooperation, the task would have been manyfold more difficult.

Finally, I am grateful to my wife, Dorothy, for her understanding and devotion throughout this undertaking, and for typing the draft copy.

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APPENDIX 1

DATA ON THE MAGNETIC FIELD

The magnet which provides this inhomogeneous field was formerly employed in the beta-ray spectrometer which was reconstructed here at the USNPGS in the period 1955-56. Although much was known about the magnet itself, there existed no data on the magnetic field until measurements were made by Kelly [5]in 1965.

This data has been compiled and is herein available for the field strength both on- and off-axis; and also, for the theoretically computed as well as experimentally measured values in Gauss.

In the diagram of the Magnetic Field Strength in this appendix, there are two values listed for each (r, z). The experimental values in the diagram are the upper ones listed in each square.

The theoretically computed values are listed in squares and are the lower values. The method by which these values were computed is as follows:

The field on-axis is given by:

$$H_0(z) = B_1 + B_2 z + B_3 z^2 + B_4 z^3 + B_5 z^4 + \ldots + B_{13} z^{12} \qquad (3\text{-}1)$$

(z expressed in meters)

where:

B(1) = 8.0498907E-02
B(2) = 2.3351831E-02
B(3) = -4.8664438E+00
B(4) = 4.2887590E+01
B(5) = -4.3626183E+02
B(6) = 3.9271101E+03
B(7) = -2.2648265E+04
B(8) = 8.2393030E+04
B(9) = -1.9359723E+05
B(10) = 2.9437706E+05
B(11) = -2.8025472E+05
B(12) = 1.5200646E+05
B(13) = -3.5865075E+04

Since A_ϕ is the only non-zero component of the vector potential, the axial component of the field strength, H_Z , can be computed and compared to values obtained by the Hall Probe.

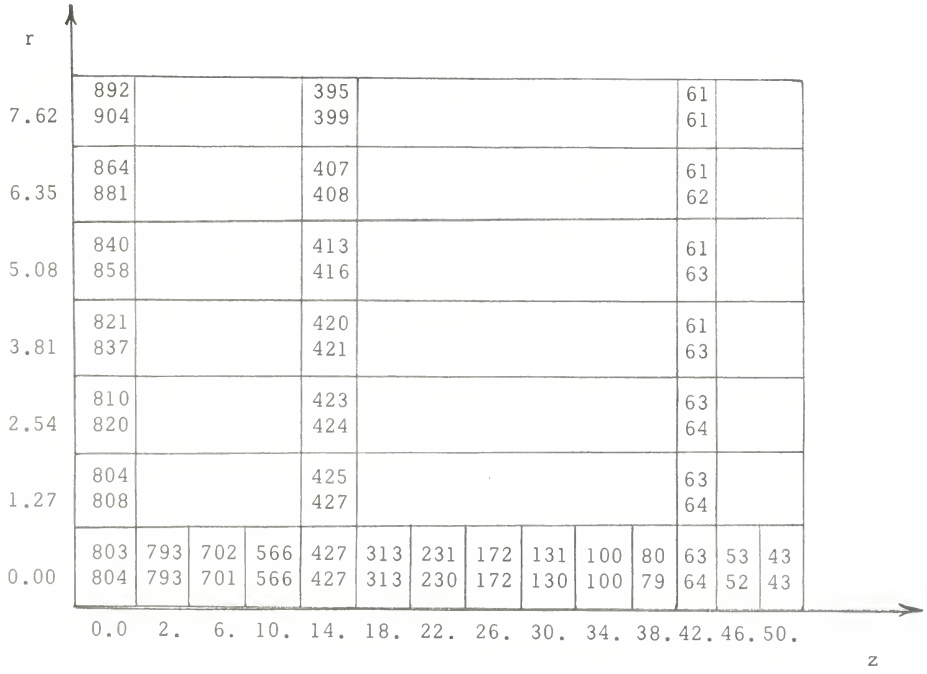
H_z becomes $\frac{1}{r}\left\{\frac{\partial}{\partial r}\left([r\ A_\phi]\right)\right\}$

where A_ϕ is equation (5-1).

And, after performing the indicated operations,

$$H_Z\ (r,z) = G_1 - \frac{r^2}{4} G_2 + \frac{r^4}{64} G_3 - \frac{r^6}{2304}\ G_4 + \ldots . \qquad (11)$$

This is demonstrated in Appendix 6.



MAGNETIC FIELD STRENGTH (in Gauss)
All distances on axes in centimeters

Upper values - experimental
Lower values - theoretical

APPENDIX 2

USEFUL FORMULAE IN CYLINDRICAL COORDINATES

Conversion from Rectangular Coordinates

$$x = r\cos\phi$$
$$y = r\sin\phi$$
$$z = z$$

The Gradient

$$\vec{\nabla}\Phi = \left(\frac{\partial\Phi}{\partial r}\right)\hat{r} + \frac{1}{r}\left(\frac{\partial\Phi}{\partial\phi}\right)\hat{\phi} + \left(\frac{\partial\Phi}{\partial z}\right)\hat{k}$$

The Divergence

$$\vec{\nabla}\cdot\vec{A} = \frac{1}{r}\left\{\frac{\partial(rAr)}{\partial r}\right\} + \frac{1}{r}\left\{\frac{\partial A\phi}{\partial\phi}\right\} + \left\{\frac{\partial Az}{\partial z}\right\}$$

The Curl

$$\vec{\nabla}\times\vec{A} = \frac{1}{r}\left[\frac{\partial Az}{\partial\phi} - \frac{\partial(rA\phi)}{\partial z}\right]\hat{r} - \left[\frac{\partial Az}{\partial r} - \frac{\partial Ar}{\partial z}\right]\hat{\phi} + \frac{1}{r}\left[\frac{\partial(rA\phi)}{\partial r} - \frac{\partial Ar}{\partial\phi}\right]\hat{k}$$

The Laplacian

$$\nabla^2\Phi = \frac{1}{r}\left\{\frac{\partial}{\partial r}\left(r\,\frac{\partial\Phi}{\partial r}\right)\right\} + \frac{1}{r^2}\left\{\frac{\partial^2\Phi}{\partial\phi^2}\right\} + \left\{\frac{\partial^2\Phi}{\partial z^2}\right\}$$

APPENDIX 3

POWER SERIES EXPANSION TO OBTAIN THE VECTOR POTENTIAL

The well known expansion, equation (5-1) will now be derived. This expression describes the vector potential for an inhomogeneous magnetic field, which acts only in the azimuthal direction. The field on-axis, $H_o(z)$, and its even derivatives can be computed.

Basically, the derivation of this expansion is as follows: Since the field is constant and involves no currents in the region of the field,

$$\vec{\nabla} \times \vec{B} = 0.$$

And,

$$\vec{B} = \vec{\nabla} \times \vec{A},$$

so that the vector equation for which a solution is desired is:

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{A}) = 0.$$

Conditions for this field are:

$$B_\phi = 0,$$

and $A_r = A_z = 0.$

In cylindrical coordinates, $\nabla \times B$ becomes

$$\vec{\nabla} \times \vec{B} = \frac{1}{r}\left[\frac{\partial B_z}{\partial \phi} - \frac{\partial (rB_\phi)}{\partial z}\right]\hat{r} - \left[\frac{\partial B_z}{\partial r} - \frac{\partial B_r}{\partial z}\right]\hat{\phi} + \frac{1}{r}\left[\frac{\partial (rB_\phi)}{\partial r} - \frac{\partial B_r}{\partial \phi}\right]\hat{z},$$

and each component must be equal to zero.

$$\frac{\partial B_z}{\partial r} = \frac{\partial B_r}{\partial z} \tag{1}$$

$$B_r = \frac{1}{r}\left[\frac{\partial A_z}{\partial \phi}\right] - \left[\frac{\partial (rA_\phi)}{\partial z}\right] = \frac{1}{r}\left\{-\frac{\partial (rA_\phi)}{\partial z}\right\} \tag{2}$$

$$B_\phi = \frac{\partial A_z}{\partial r} - \frac{\partial A_r}{\partial z} \equiv 0$$

$$B_z = \frac{1}{r}\left[\frac{\partial (rA_\phi)}{\partial r}\right] - \frac{\partial A_r}{\partial \phi} = \frac{1}{r}\left\{\frac{\partial (rA_\phi)}{\partial r}\right\} \tag{3}$$

From equations 1, 2 and 3,

$$\frac{\partial}{\partial r}\left[\frac{1}{r}\left\{\frac{\partial}{\partial r}(rA)\right\}\right] = \frac{\partial}{\partial z}\left[\frac{1}{r}\left\{-\frac{\partial}{\partial z}(rA)\right\}\right] \quad \text{, and}$$

$$\frac{\partial}{\partial r}\left[\frac{1}{r}\left\{r\frac{\partial A}{\partial r} + A\right\}\right] + \frac{\partial}{\partial z}\left[\frac{1}{r}\left\{\frac{\partial r}{\partial z}A + r\frac{\partial A}{\partial z}\right\}\right] = 0, \text{ and}$$

$$\frac{\partial}{\partial r}\left[\frac{\partial A}{\partial r} + \frac{A}{r}\right] + \frac{\partial}{\partial z}\left[\frac{\partial r}{\partial z}\frac{A}{r} + \frac{\partial A}{\partial z}\right] = 0,$$

and the partial derivative $\frac{\partial r}{\partial z}$ is zero as the coordinates are independent.

Thus,

$$\frac{\partial^2 A}{\partial r^2} + \frac{1}{r}\frac{\partial A}{\partial r} - \frac{A}{r^2} + \frac{\partial^2 A}{\partial z^2} = 0.$$

Here, a solution is assumed in the form $\sum_{n=0}^{\infty} a_n(z)\, r^n$ where the coefficients $a_n(z)$ are differentiable. To determine the coefficients,

$$\frac{\partial A}{\partial r} = \Sigma\, n\, a_n(z)\, r^{n-1},$$

and

$$\frac{\partial^2 A}{\partial r^2} = \Sigma\, n(n-1) a_n(z)\, r^{n-2},$$

and

$$\frac{\partial A}{\partial z} = \Sigma\, a_n'(z) r^n,$$

and

$$\frac{\partial^2 A}{\partial z^2} = \Sigma\, a_n''(z)\, r^n$$

Substituting in, and multiplying through by r^2

$$\Sigma(n)(n-1)a_n(z)r^n + \Sigma n\, a_n(z)r^n - \Sigma a_n(z)r^n + \Sigma a_n''(z)r^{n+2} = 0$$

$$\Sigma\,\{n(n-1) + n - 1\}a_n(z)r^n = -\Sigma\, a_n''(z)r^{n+2}$$

For n=0, the left hand side of the last equation reduces to $-a_o(z)$, and there exists no n=1 term. Therefore,

$$-a_o(z) + \sum_{n=2}^{\infty} \{n(n-1) + n-1\} a_n(z) r^n + \sum_{n=0} a_n''(z) r^{n+2} = 0$$

$$-a_o(z) + \sum_{n=0}^{\infty} \{(n+2)(n+1)+n+1\} a_{n+2}(z) r^{n+2} + \sum_{n=0}^{\infty} a_n''(z) r^{n+2} = 0$$

$$-a_o(z) + \sum_{n=0}^{\infty} \{(n+3)(n+1)\} a_{n+2}(z) r^{n+2} + \sum_{n=0}^{\infty} a_n''(z) r^{n+2} = 0$$

$$-a_o(z) + \sum_{n=0}^{\infty} \{[(n+3)(n+1)] a_{n+2}(z) + a_n''(z)\} r^{n+2} = 0$$

The following must then be true, as for all power series expansions:

$a_o(z) \equiv 0$, hence

$$(n+3)(n+1) a_{n+2}(z) + a_n''(z) = 0$$

$$\therefore a_{n+2}(z) = \frac{-a_n''(z)}{(n+3)(n+1)}$$

Whence, a recursion relationship yields the important needed parameters. Obviously, there can be no terms for n even.

For $n = 1$ $\quad a_3(z) = \dfrac{-a_1''(z)}{8}$

$n = 3$ $\quad a_5(z) = \dfrac{-a_3''(z)}{24}$, etc.

As $A(r,z) = \sum_{n=0}^{\infty} a_n(z) r^n$

$$= a_1(z)r + a_3(z)r^3 + a_5(z)r^5 + a_7(z)r^7 + \ldots$$

Making the substitutions,

$$A = a_1(z)r - a_1''(z)\frac{r^3}{8} + \left(\frac{1}{24}\right)\left(\frac{1}{8}\right) a_1''''(z) r^5 - \ldots$$

And, to evaluate $a_1(z)$, solve for B_Z using $\nabla \times A$,

$$B_Z = \frac{1}{r} \cdot \frac{\partial (rA)}{\partial r} = 2a_1(z) - \frac{4}{8} a_1''(z) r^2 + \frac{6}{248} a_1''''(z) r^4 - \ldots$$

Knowing that B_z is equal to $H_o(z)$ for $r = 0$, hence,

$$H_o(z) = B_z(r=0) = 2a_1(z), \qquad \therefore a_1(z) = \tfrac{1}{2} H_o(z)$$

and the expression for the Vector Potential is obtained as

$$A(r,z) = \frac{r}{2} H_o(z) - \frac{r^3}{16} H_o''(z) + \frac{r^5}{384} H_o''''(z) - \ldots \quad .$$

APPENDIX 4

THE DIFFERENTIAL EQUATION DEVELOPMENT

The essentials of this operation involve simply applying Newton's second law in cylindrical coordinates to the magnetic force acting on the particle. Finally, time and the azimuthal variables can be eliminated by means of the two motion constants, energy and the canonically conjugate angular momentum. Since the particle will begin its trajectory on the z-axis, the canonically conjugate angular momentum is, in fact, zero.

Applying Newton's 2nd law,

$$\vec{F}_{mag} = q(\vec{v} \times \vec{B}) = m(\vec{a})$$

where

$$\vec{a} \equiv \frac{d}{dt} [\vec{v}]$$

In cylindrical coordinates, the velocity vector is

$$\vec{v} = \dot{r}\,\hat{r} + r\dot{\phi}\,\hat{\phi} + \dot{z}\,\hat{z},$$

and, the acceleration vector is

$$\vec{a} = (\ddot{r} - r\dot{\phi}^2)\,\hat{r} + (2\dot{r}\dot{\phi} + r\ddot{\phi})\,\hat{\phi} + (\ddot{z})\,\hat{z}.$$

Knowing the vector potential, the magnetic field $\vec{B}$ and the quantity $\vec{v} \times \vec{B}$ can be found.

$$\vec{B} \equiv \vec{\nabla} \times \vec{A} = \frac{1}{r}\left[\frac{\partial}{\partial \phi}(Az) - \frac{\partial}{\partial z}(r A_\phi)\right]\hat{r} + \left[\frac{\partial}{\partial r}(Az) - \frac{\partial}{\partial z}(Ar)\right]\hat{\phi} + \frac{1}{r}\left[\frac{\partial}{\partial r}(r A_\phi) - \frac{\partial}{\partial \phi}(Ar)\right]\hat{z}$$

But: $\vec{A} = A_\phi\,\hat{\phi}$,

$Ar = Az = 0$

and,

$$\vec{B} = \frac{1}{r}\left[-\frac{\partial}{\partial z}(rA_\phi)\right]\hat{r} + \frac{1}{r}\left[\frac{\partial}{\partial r}(rA_\phi)\right]\hat{z}.$$

Hence:

$$\vec{v} \times \vec{B} = \left[\dot{\phi} \frac{\partial}{\partial r}\left(rA_\phi\right)\right]\hat{r} + \left[-\frac{\dot{r}}{r}\frac{\partial}{\partial r}\left(rA_\phi\right) - \frac{\dot{z}}{r}\frac{\partial}{\partial z}\left(rA_\phi\right)\right]\hat{\phi} + \left[\dot{\phi}\frac{\partial}{\partial z}\left(rA_\phi\right)\right]\hat{z}.$$

Equating each orthogonal cylindrical component, the following is obtained,

$$m(\ddot{r} - r\dot{\phi}^2) = q(\dot{\phi}\frac{\partial}{\partial r} rA_\phi), \tag{4}$$

$$m(2\dot{r}\dot{\phi} + r\ddot{\phi}) = q\left[-\frac{\dot{r}}{r}\frac{\partial}{\partial r}\left(rA_\phi\right) - \frac{\dot{z}}{r}\frac{\partial}{\partial z}\left(rA_\phi\right)\right], \tag{5}$$

$$m(\ddot{z}) = q(\dot{\phi}\frac{\partial}{\partial z} rA_\phi). \tag{6}$$

These three equations can be reduced further to:

$$\frac{d}{dt}(m\dot{r}) = mr\dot{\phi}^2 + q\dot{\phi}\frac{\partial}{\partial r}(rA_\phi),$$

$$\frac{d}{dt}(mr^2\dot{\phi} + qrA_\phi) = 0,$$

and

$$\frac{d}{dt}(m\dot{z}) = qr\dot{\phi}\frac{\partial}{\partial z}(A_\phi).$$

From the middle equation above, it can be shown that the quantity conserved is the canonically conjugate angular momentum about the symmetry axis. Thus,

$$p_c \equiv mr^2\dot{\phi} + qrA_\phi,$$

$$\dot{\phi} = \frac{p_c - qrA_\phi}{mr^2}$$

and,

$$\frac{d}{dt}(m\dot{r}) = \frac{q^2}{m}\left[\frac{p_c}{qr} - A_\phi\right]\left[\frac{p_c}{qr^2} + \frac{\partial A_\phi}{\partial r}\right]$$

$$\frac{d}{dt}(m\dot{z}) = \frac{q^2}{m}\left[\frac{\partial A_\phi}{\partial z}\right]\left[\frac{p_c}{rq} - A_\phi\right].$$

Replacing the independent variable of time (t) with the distance on the z-axis (z) yields

$$v^2 = \left[\left(\frac{\partial r}{\partial z}\right)^2 + 1\right](\dot{z})^2 + r^2\left[\frac{p_c - qrA\,\phi}{mr^2}\right]^2 \qquad (7)$$

and

$$(\dot{z})^2 = \frac{v^2 - \frac{q^2}{m^2}\left[\frac{p_c}{qr} - A\,\phi\right]^2}{\left\{1 + \left(\frac{dr}{dz}\right)^2\right\}}$$

This operation can be performed as follows:

$$\frac{d}{dt}(m\dot{r}) = \dot{z}\left[\frac{d}{dz}\left(m\frac{dr}{dz}\dot{z}\right)\right],$$

$$\frac{d}{dt}(m\dot{z}) = \dot{z}\left[\frac{\partial}{\partial z}(m\dot{z})\right],$$

$$\vec{v} = \dot{r}\,\hat{r} + r\dot{\phi}\,\hat{\phi} + \dot{z}\,\hat{z},$$

$$v^2 = \vec{v}\cdot\vec{v} = (\dot{r})^2 + (r\dot{\phi})^2 + (\dot{z})^2,$$

and

$$\dot{r} = \frac{dr}{dz}\dot{z},$$

$$\dot{\phi} = \frac{p_c - qrA}{mr^2}.$$

Hence:

$$v^2 = \left[\left(\frac{dr}{dz}\right)^2 + 1\right](\dot{z})^2 + r^2\left[\frac{p_c - qrA}{mr^2}\right]^2$$

$$= \left[1 + \left(\frac{dr}{dz}\right)^2\right](\dot{z})^2 + \frac{q^2}{m^2}\left[\frac{p_c}{qr} - A\right]^2.$$

Further:

$$(\dot{z})^2 = \frac{v^2 - \left(\frac{q}{m}\right)^2\left[\frac{p_c}{qr} - A\right]^2}{\left[1 + \left(\frac{dr}{dz}\right)^2\right]}, \qquad (8)$$

and:

$$m \frac{d^2r}{dz^2}(\dot{z})^2 + \frac{dr}{dz}\left[m\dot{z} \frac{d}{dz}(\dot{z}) \right] = \frac{q^2}{m} \left\{ \frac{p_c}{qr} - A \right\} \left[\frac{p_c}{qr^2} + \frac{\partial A}{\partial r} \right] \quad (9)$$

$$m(\dot{z}) \left[\frac{d}{dz}(z) \right] = \frac{q^2}{m} \left\{ \frac{\partial A}{\partial z} \right\} \left[\frac{p_c}{qr} - A \right] . \quad (10)$$

Combining the remaining equations 8, 9, and 10, and then allowing that

$$p_c \equiv 0$$

and

$$k \equiv \frac{mv}{q} ,$$

the following equation results:

$$\frac{r''}{[1 + (r')^2]} \left\{ k^2 - A_\phi^2 \right\} - r' \left[\left(A_\phi \right) \frac{\partial A_\phi}{\partial z} \right] + \left\{ \left(A_\phi \right) \frac{\partial A_\phi}{\partial r} \right\} = 0 \quad (4\text{-}1)$$

where the dots throughout this discussion indicate derivatives with respect to time, and the primes indicate derivatives with respect to the variable z. [4]

APPENDIX 5

DEVELOPMENT OF THE VECTOR POTENTIAL

To adequately describe the field at every point, and for use in the general trajectory previously derived, equation (4-1), the following quantities are needed:

$\vec{A}$ = The Vector Potential,

$\frac{\partial \vec{A}}{\partial z}$ = The first partial derivative of A with respect to z,

and

$\frac{\partial \vec{A}}{\partial r}$ = The first partial derivative of A with respect to r.

The vector potential, found by the power series expansion in Appendix 3, is

$$A = \frac{r}{2}[G_1] - \frac{r^3}{16}[G_2] + \frac{r^5}{384}[G_3] - \frac{r^7}{18432}[G_4] + \ldots + \frac{r^{13}}{29727129600}[G_7],$$

where, for the purposes of programming, the G functions are defined as follows:

$$G_1 \equiv H_0(z)$$

$$G_2 \equiv \frac{\partial^2 H_0(z)}{\partial z^2}$$

$$G_3 \equiv \frac{\partial^4 H_0}{\partial z^4}$$

$$G_5 \equiv \frac{\partial^6 H_0}{\partial z^6}$$

$$\vdots$$

$$G_7 \equiv \frac{\partial^{12} H_0}{\partial z^{12}} .$$

The first partial of $\vec{A}$ with respect to r becomes,

$$\frac{\partial \vec{A}}{\partial r} = \tfrac{1}{2}[G_1] - \frac{3r^2}{16}[G_2] + \frac{5r^4}{384}[G_3] - \frac{7r^6}{18432}[G_4] + \frac{9r^8}{1474560}[G_5]$$

$$- \frac{11r^{10}}{176047200}[G_6] + \frac{13r^{12}}{29727129600}[G_7]$$

The first partial of A with respect to z is a little more tedious, but can be shown to be,

$$\frac{\partial \vec{A}}{\partial z} = \frac{r}{2}[F_1] - \frac{r^3}{16}[F_2] + \frac{r^5}{384}[F_3] - \ldots\ldots[F_6]$$

where the F functions are defined as follows (again for programming convenience),

$$F_1 \equiv \frac{\partial G_1}{\partial z}$$

$$F_2 \equiv \frac{\partial G_2}{\partial z}$$

$$F_3 \equiv \frac{\partial G_3}{\partial z}$$

$$F_4 \equiv \frac{\partial G_4}{\partial z}$$

$$F_5 \equiv \frac{\partial G_5}{\partial z}$$

$$F_6 \equiv \frac{\partial G_6}{\partial z}$$

$$F_7 = 0.$$

APPENDIX 6

PERTINENT MACHINE PROGRAMS

The pertinent computer programs used in the solution of this problem are listed in this appendix in the following manner:

Program A - Least-squares polynomial generation by the PROGRAM CURVE, and contains 7 pages.

Program B - Theoretical off-axis field check labeled PROGRAM WATCHOUT, and contains 2 pages.

Program C - The main trajectory program labeled PROGRAM ORBITS, and contains 15 pages.

Reverse Blank

```
      PROGRAM CURVE
      DIMENSION X(18), F2(18), W(18), Y(18), DELY(18), B(18), SB(18), T(
     118), ST(18), C(18), CT(18), A(30,30)
      READ 1 (X(I),I=1,18)
    1 FORMAT (18F4.0)
      READ 200,(F2(I),I=1,18)
  200 FORMAT(12F6.4)
      CALL LSQPOL (18,12,0,0,0,SIGMA,X,F2,W,Y,DELY,B,SB,T,ST,C,CT,A)
      DO 10 I=1,18
   10 PRINT 2, I,B(I)
    2 FORMAT (15,3X,4H B =F 5.7)
      END
      SUBROUTINE LSQPOL(M,KM,IW,ISW,LP,SIGMA,X,F2,W,Y,DELY,B,SB,T,ST,C, 00000000
     1SC,A)                                                             000   10
      DIMENSION S(30),X(1),F2(1),ST(1),SB(1),F(100),PM(100),P(100),B(1),00000020
     1DELY(1),W(1),A(30,30),T(1),Y(1),BM(11,11),D(11,11),C(1),SC(1)     00000030
      LL=0                                                                   40
    9 FM=0.0                                                            000   50
      A(1,1)=1.0                                                        000   60
      A(2,2)=1.0                                                        000*  70
      FBAR=0.0                                                          000   80
      XBAR=0.0                                                          000   90
      DO10I=1,M                                                         00000100
      IF(IW)1009,1010,1009                                              00000110
 1010 W2=1.0                                                            000* 120
      W(I)=1.0                                                          00000130
      GOTO1011                                                          00000140
 1009 W2=SQRTF(W(I))                                                    00000150
 1011 FM=FM+W(I)                                                        00000160
      F(I)=W2*F2(I)                                                     00000170
      PM(I) = W2                                                        00000180
      FBAR=FBAR+F(I)*PM(I)                                              00000190
   10 XBAR=XBAR+X(I)*PM(I)**2                                           00000200
      XBAR=XBAR/FM                                                      00000210
      T(1)=FBAR/FM                                                      00000220
      A(2,1)=-XBAR                                                      00000230
```

```
      PXF=0.0                                                    00000240
      PXP=0.0                                                    0000 250
      DO20I=1,M                                                  00000260
      P(I)=(X(I)-XBAR)*PM(I)                                     00000270
      PXF=PXF+P(I)*F(I)                                          00000280
   20 PXP=PXP+P(I)*P(I)                                          00000290
      T(2)=PXF/PXP                                               00000300
      PMXPM=FM                                                   00000310
      S(1)=PMXPM                                                 00000320
      KM=KM+1                                                    00000330
      B(1)=T(1)*A(1,1)+T(2)*A(2,1)                               00000340
      B(2)=T(2)*A(2,2)                                           00000350
   60 DO190K=2,KM                                                00000360
      IF(K-2)40,165,65                                           00000370
   40 PRINT 4000                                                 0000 380
 4000 FORMAT(7HSTOP 40)                                          00000390
      STOP                                                       000  400
   65 XPXP=0.0                                                   00000410
      XPXPM=0.0                                                  00000420
      B(K)=0.0                                                   00000430
      DO70J=1,M                                                  00000440
      XP=X(J)*P(J)                                               00000450
      XPXP=XPXP+XP*P(J)                                          00000460
   70 XPXPM=XPXPM+XP*PM(J)                                       00000470
      ALPHA=XPXP/PXP                                             00000480
      BETA=XPXPM/PMXPM                                           00000490
      PPXF=0.0                                                   00000500
      PPXPP=0.0                                                  00000510
      DO90I=1,M                                                  00000520
   80 PT=P(I)                                                    00000530
   81 P(I)=X(I)*PT-ALPHA*PT-BETA*PM(I)                           00000540
   82 PPXF=PPXF+P(I)*F(I)                                        00000550
   83 PPXPP=PPXPP+P(I)*P(I)                                      00000560
   90 PM(I)=PT                                                   00000570
      T(K)=PPXF/PPXPP                                            00000580
      PMXPM=PXP                                                  00000590
```

```
      PXP=PPXPP                                                          00000600
      A(K,1)=-ALPHA*A(K-1,1)-BETA*A(K-2,1)                               00000610
      A(K,K-1)=A(K-1,K-2)-A(K-1,K-1)*ALPHA                               00000620
      A(K,K)=1.0                                                         00000630
      IF(K-3)150,150,110                                                 00000640
  110 K1=K-2                                                             00000650
      DO120I=2,K1                                                        00000660
  120 A(K,I)=A(K-1,I-1)-ALPHA*A(K-1,I)-BETA*A(K-2,I)                     00000670
  150 DO160I=1,K                                                         00000680
  160 B(I)=B(I)+T(K)*A(K,I)                                              00000690
  165 SIG3=0.0                                                           00000700
      DO180I=1,M                                                         00000710
      Y(I)=POLYE1(X(I),K,B)                                              00000720
  175 DELY(I)=Y(I)-F2(I)                                                 00000730
  180 SIG3 = SIG3 + (DELY(I)**2)*W(I)                                    00000740
      SIG2 = SIG3/FLOATF(M-K)                                            00000750
      IF(K-2)40,1650,1651                                                00000760
 1650 FLEV = 0.                                                          00000770
      GO TO 1652                                                         00000780
 1651 FLEV = (SUMDEV2 - SIG3)/SIG2                                       00000790
 1652 SUMDEV2 = SIG3                                                     00000800
      SIGMA=SQRTF(SIG2)                                                  00000810
      S(K) = PXP                                                         00000820
      DO499I=1,K                                                         00000830
  499 ST(I)=SIGMA/SQRTF(S(I))                                            00000840
      DO501I=1,K                                                         00000850
      SB(I)=0.0                                                          00000860
      DO500J=I,K                                                         00000870
  500 SB(I)=SB(I)+(A(J,I)*ST(J))**2                                      00000880
  501 SB(I)=SQRTF(SB(I))                                                 00000890
      IF(LP)658,183,658                                                  00000900
  658 IF(K-2)652,651,652                                                 00000910
  651 D(1,1)=1.0                                                         00000920
      D(2,2)=1.0                                                         00000930
      D(2,1)=0.0                                                         00000940
      D(3,3)=3./2.                                                       00000950
```

```
D(3,2)=0.                                                    00000960
D(3,1)=-1./2.                                                00000970
D(4,4)=5./2.                                                 00000980
D(4,3)=0.                                                    00000990
D(4,2)=-3./2.                                                00001000
D(4,1)=0.                                                    00001010
D(5,5)=35./8.                                                00001020
D(5,4)=0.                                                    00001030
D(5,3)=-30./8.                                               00001040
D(5,2)=0.                                                    00001050
D(5,1)=3./8.                                                 00001060
D(6,6)=63./8.                                                00001070
D(6,5)=0.                                                    00001080
D(6,4)=-70./8.                                               00001090
D(6,3)=0.                                                    00001100
D(6,2)=15./8.                                                00001110
D(6,1)=0.                                                    00001120
D(7,7)=231./16.                                              00001130
D(7,6)=0.                                                    00001140
D(7,5)=-315./16.                                             00001150
D(7,4)=0.                                                    00001160
D(7,3)=105./16.                                              00001170
D(7,2)=0.                                                    00001180
D(7,1)=-5./16.                                               00001190
D(8,8)=429./16.                                              00001200
D(8,7)=0.                                                    00001210
D(8,6)=-693./16.                                             00001220
D(8,5)=0.                                                    00001230
D(8,4)=315./16.                                              00001240
D(8,3)=0.                                                    00001250
D(8,2)=-35./16.                                              00001260
D(8,1)=0.                                                    00001270
D(9,9)=6435./128.                                            00001280
D(9,8)=0.                                                    00001290
D(9,7)=-12012./128.                                          00001300
D(9,6)=0.                                                    00001310
```

```
      D(9,5)=6930./128.                                          00001320
      D(9,4)=0.                                                  00001330
      D(9,3)=-1260./128.                                         00001340
      D(9,2)=0.                                                  00001350
      D(9,1)=35./128.                                            00001360
      D(10,10)=12155./128.                                       00001370
      D(10,9)=0.                                                 00001380
      D(10,8)=-25740./128.                                       00001390
      D(10,7)=0.                                                 00001400
      D(10,6)=18018./128.                                        00001410
      D(10,5)=0.                                                 00001420
      D(10,4)=-4620./128.                                        00001430
      D(10,3)=0.                                                 00001440
      D(10,2)=315./128.                                          00001450
      D(10,1)=0.                                                 00001460
      D(11,11)=46189./256.                                       00001470
      D(11,10)=0.                                                00001480
      D(11,9)=-109395./256.                                      00001490
      D(11,8)=0.                                                 00001500
      D(11,7)=90090./256.                                        00001510
      D(11,6)=0.                                                 00001520
      D(11,5)=-30030./256.                                       00001530
      D(11,4)=0.                                                 00001540
      D(11,3)=3465./256.                                         00001550
      D(11,2)=0.                                                 00001560
      D(11,1)=-63./256.                                          00001570
  652 DO700II=1,K                                                00001580
      J=K-II+1                                                   00001590
      VARA=0.0                                                   00001600
      III=K-J                                                    00001610
      IF(III)702,701,702                                         00001620
  702 DO703JJ=1,III                                              00001630
      JK=K-JJ+1                                                  00001640
  703 VARA=VARA+D(JK,J)*BM(K,JK)                                 00001650
  701 BM(K,J)=(A(K,J)-VARA)/D(J,J)                               00001660
      IF(K-2)700,704,700                                         00001670
```

```
704 BM(1,1)=A(1,1)/D(1,1)                                                00001680
700 CONTINUE                                                             00001690
705 DO708I=1,K                                                           00001700
    C(I)=0.0                                                             00001710
    SC(I)=0.0                                                            00001720
    DO707J=1,K                                                           00001730
    C(I)=C(I)+BM(J,I)*T(J)                                               00001740
707 SC(I)=SC(I)+(BM(J,I)*ST(J))**2                                       00001750
708 SC(I)=SQRTF(SC(I))                                                   00001760
183 CONTINUE                                                             00001770
192 PRINT 600                                                            00001780
    PRINT 1,(I,B(I),SB(I),I=1,K)                                         00001790
185 PRINT 186,SIGMA,FLEV,SUMDEV2                                         00001800
    PRINT 601,(I,T(I),ST(I),I=1,K)                                       00001810
    IF(LP)187,670,187                                                    00001820
187 PRINT 188                                                            00001830
    PRINT 602,(I,C(I),SC(I),I=1,K)                                       00001840
670 PRINT 2                                                              00001850
    PRINT 603,(I,X(I),F2(I),Y(I),DELY(I),W(I),I=1,M)                     00001860
190 CONTINUE                                                             00001870
211 IF(ISW) 210,220,210                                                  00001880
210 DO215I=2,KM                                                          00001890
215 PRINT 5,I,(A(I,J),J=1,I)                                             00001900
220 KM=KM-1                                                              00001910
    RETURN                                                               00001920
  1 FORMAT(3H B(0PI2,2H)=1PE15.7,6H ERRB=E10.3,3H B(0PI2,2H)=1PE15.7,     00001930
   16H ERRB=E10.3,3H B(0PI2,2H)=1PEI5.7,6H ERRB=E10.3)                   00001940
  2 FORMAT(4H0  I 11X 4HX(I) 12X4HF(I)12X4HY(I)12X7HDELY(I)10X4HW(I)/)   00001950
  5 FORMAT(36H0 ORTHOGONAL POLYNOMIAL COEFF FOR K=I5//(1P8E15.6))        00001960
186 FORMAT(7H0SIGMA=1PE16.7,9H F LEVEL=1PE16.7,12H SUM SQ DEV=,1PE16.700001970
   *                    //  45H COEFFICIENTS OF Y=T1*P1+T2*P2+ETC AND00001980
   1 ERRORS/)                                                            00001990
188 FORMAT(23H0  LEGENDRE POLYNOMIALS/45H COEFFICIENTS OF Y=C1*L1+C2*L00002000
   12+ETC AND ERRORS/)                                                   00002010
600 FORMAT(41H1COEFFICIENTS OF Y=B1+B2*X+ETC AND ERRORS/)                00002020
601 FORMAT(3H T(I2,2H)=1PE15.7,6H ERRT=E10.3,3H T(0PI2,2H)=1PE15.7,6H    00002030
```

```
     1ERRT=E10.3,3H T(0PI2,2H)=1PE15.7,6H ERRT=E10.3)                                  00002040
  602 FORMAT(3H C(I2,2H)=1PE15.7,6H ERRC=E10.3,3H C(0PI2,2H)=1PE15.7,6H               00002050
     1ERRC=E10.3,3H C(0PI2,2H)=1PE15.7,6H ERRC=E10.3)                                 00002060
  603 FORMAT(I6,1P5E16.7)                                                             00002070
      END                                                                             00002080
      FUNCTION POLYE1(X,K,B)                                                          00002090
      DIMENSION B(30)                                                                 00002100
   10 S=B(K)                                                                          00002110
      KK=K-1                                                                          00002120
   20 DO 40 I=1,KK                                                                    00002130
   30 IK=K-I                                                                          00002140
   40 S=X*S+B(IK)                                                                     00002150
      POLYE1=S                                                                        00002160
       END                                                                            00002170
      END

.00 .02 .06 .10 .14 .18 .22 .26 .30 .34 .38 .42 .46 .50 .54 .58 .62 .66
  805   793   702   566   428   313   230   172   131   100    80    64
   53    43    36    31    26    24
```

```
      PROGRAM WATCHOUT
      DIMENSION G(20),B(20),ZZ(20),RR(20),H(20,20)
      B( 1)=  8.0498907E-02
      B( 2)=  2.3351831E-02
      B( 3)= -4.8664438E+00
      B( 4)=  4.2887590E+01
      B( 5)= -4.3626183E+02
      B( 6)=  3.9271101E+03
      B( 7)= -2.2648265E+04
      B( 8)=  8.2393030E+04
      B( 9)= -1.9359723E+05
      B(10)=  2.9437706E+05
      B(11)= -2.8025472E+05
      B(12)=  1.5200646E+05
      B(13)= -3.5865075E+04
      ZZ(1)=-0.00
      ZZ(2)=-0.14
      RR(1)=.0
      RR(2)=0.0127
      RR(3)=0.0254
      RR(4)=0.0381
      RR(5)=0.0508
      RR(6)=0.0635
      RR(7)=0.0762
      DO 10 I=1,3
      Z=ZZ(I)
      G(1)=B(1)+B(2)*Z+B(3)*Z**2+B(4)*Z**3+B(5)*Z**4+B(6)*Z**5+B(7)*Z**6
     1+B(8)*Z**7+B(9)*Z**8+B(10)*Z**9+B(11)*Z**10+B(12)*Z**11+B(13)*Z**1
     22
      G(2)=2.*B(3)+6.*B(4)*Z+12.*B(5)*Z**2+20.*B(6)*Z**3+30.*B(7)*Z**4+4
     12.*B(8)*Z**5+56.*B(9)*Z**6+72.*B(10)*Z**7+90.*B(11)*Z**8+110.*B(12
     2)*Z**9+132.*B(13)*Z**10
      G(3)=24.*B(5)+120.*B(6)*Z+360.*B(7)*Z**2+840.*B(8)*Z**3+1680.*B(9)
     1*Z**4+3024.*B(10)*Z**5+5040.*B(11)*Z**6+7920.*B(12)*Z**7+11880.*B(
     213)*Z**8
      G(4)=720.*B(7)+5040.*B(8)*Z+20160.*B(9)*Z**2+60480.*B(10)*Z**3+151
```

```
     1200.*B(11)*Z**4+332640.*B(12)*Z**5+665280.*B(13)*Z**6
      G(5)=40320.*B(9)+362880.*B(10)*Z+1814400.*B(11)*Z**2+6652800.*B(12
     1)*Z**3+19958400.*B(13)*Z**4
      G(6)=3628800.*B(11)+39916800.*B(12)*Z+239500800.*B(13)*Z**2
      G(7)=479001600.*B(13)
      PRINT 30, (G(KK),KK=1,7)
      DO 10 J=1,7
      R=RR(J)
      H(I,J)=G(1)-G(2)*R**2/4.+G(3)*R**4/64.-G(4)*R**6/2304.+G(5)*R**8/1
     147456.-G(6)*R**10/14745600.+G(7)*R**12/2123366400.
   10 CONTINUE
      PRINT 20,(ZZ(I),I=1,3)
   20 FORMAT (1H1///,15X,7E15.8)
      DO 40 J=1,7
      PRINT 30,RR(J),(H(I,J),I=1,3)
   30 FORMAT (//8E15.8)
   40 CONTINUE
      END
      END
```

```
      PROGRAM ORBITS
      DIMENSION X(30),XDOT(30),C(15),B(15),F(15),G(15)
      C(10)=1
    1 CALL INTEG1(T,X,XDOT,C)
C     ENER=ENERGY OF THE H2 ION IN ELECTRON-VOLTS
      ENER=C(1)
C     OKAY=(MOM/CHARGE)*(MOM/CHARGE)
      OKAY=(4.17576E-08)*(ENER)
C     P IS THE DECIMAL FRACTION OF THE MAG FLD CURRENT DESIRED
      P=C(2)
      B( 1)=  8.0498907E-02
      B( 2)=  2.3351831E-02
      B( 3)= -4.8664438E+00
      B( 4)=  4.2887590E+01
      B( 5)= -4.3626183E+02
      B( 6)=  3.9271101E+03
      B( 7)= -2.2648265E+04
      B( 8)=  8.2393030E+04
      B( 9)= -1.9359723E+05
      B(10)=  2.9437706E+05
      B(11)= -2.8025472E+05
      B(12)=  1.5200646E+05
      B(13)= -3.5865075E+04
      F(1)=B(2)+2.*B(3)*T+3.*B(4)*T**2+4.*B(5)*T**3+5.*B(6)*T**4+6.*B(7)
     1*T**5+7.*B(8)*T**6+8.*B(9)*T**7+9.*B(10)*T**8+10.*B(11)*T**9+11.*B
     2(12)*T**10+12.*B(13)*T**11
      F(2)=6.*B(4)+24.*B(5)*T+60.*B(6)*T**2+120.*B(7)*T**3+210.*B(8)*T**
     14+336.*B(9)*T**5+504.*B(10)*T**6+720.*B(11)*T**7+990.*B(12)*T**8+1
     22320.*B(13)*T**9
      F(3)=120.*B(6)+720.*B(7)*T+2520.*B(8)*T**2+6720.*B(9)*T**3+15120.*
     1B(10)*T**4+30240.*B(11)*T**5+55440.*B(12)*T**6+95040.*B(13)*T**7
      F(4)=5040.*B(8)+40320.*B(9)*T+181440.*B(10)*T**2+604800.*B(11)*T**
     13+1663200.*B(12)*T**4+3991680.*B(13)*T**5
      F(5)=362880.*B(10)+3628800.*B(11)*T+19958400.*B(12)*T**2+79833600.
     1*B(13)*T**3
      F(6)=39916800.*B(12)+479001600.*B(13)*T
```

```
      VECDZ=X(1)*F(1)/2.-F(2)*X(1)**3/16.+F(3)*X(1)**5/384.-F(4)*X(1)**7
     1/18432.+F(5)*X(1)**9/1474560.-F(6)*X(1)**11/176947200.
      G(1)=B(1)+B(2)*T+B(3)*T**2+B(4)*T**3+B(5)*T**4+B(6)*T**5+B(7)*T**6
     1+B(8)*T**7+B(9)*T**8+B(10)*T**9+B(11)*T**10+B(12)*T**11+B(13)*T**1
     122
      G(2)=2.*B(3)+6.*B(4)*T+12.*B(5)*T**2+20.*B(6)*T**3+30.*B(7)*T**4+4
     12.*B(8)*T**5+56.*B(9)*T**6+72.*B(10)*T**7+90.*B(11)*T**8+110.*B(12
     2)*T**9+132.*B(13)*T**10
      G(3)=24.*B(5)+120.*B(6)*T+360.*B(7)*T**2+840.*B(8)*T**3+1680.*B(9)
     1*T**4+3024.*B(10)*T**5+5040.*B(11)*T**6+7920.*B(12)*T**7+11880.*B(
     213)*T**8
      G(4)=720.*B(7)+5040.*B(8)*T+20160.*B(9)*T**2+60480.*B(10)*T**3+151
     1200.*B(11)*T**4+332640.*B(12)*T**5+665280.*B(13)*T**6
      G(5)=40320.*B(9)+362880.*B(10)*T+1814400.*B(11)*T**2+6652800.*B(12
     1)*T**3+19958400.*B(13)*T**4
      G(6)=3628800.*B(11)+39916800.*B(12)*T+239500800.*B(13)*T**2
      G(7)=479001600.*B(13)
      VECDR=G(1)/2.-3.*G(2)*X(1)**2/16.+5.*G(3)*X(1)**4/384.-7.*G(4)*X(1
     1)**6/18432.+9.*G(5)*X(1)**8/1474560.-11.*G(6)*X(1)**10/176947200.+
     213.*G(7)*X(1)**12/29727129600.
      VECPT=X(1)*G(1)/2.-G(2)*X(1)**3/16.+G(3)*X(1)**5/384.-G(4)*X(1)**7
     1/18432.+G(5)*X(1)**9/1474560.-G(6)*X(1)**11/176947200.+G(7)*X(1)**
     213/29727129600.
      FUNC1=OKAY-VECPT*VECPT*P*P
      FUNC2=VECPT*VECDZ*P*P
      FUNC3=VECPT*VECDR*P*P
      FUNC4=(FUNC2)/(FUNC1)
      FUNC5=(FUNC3)/(FUNC1)
      XDOT(2)=X(2)*(FUNC4)+X(2)*X(2)*X(2)*(FUNC4)-X(2)*X(2)*(FUNC5)-(FUN
     1C5)
      XDOT(1)=X(2)
      GO TO 1
      END
      SUBROUTINE INTEG1 (TC, XC, DX, C)                                  00000000
*                                                                         0    10
C          SUBROUTINE USES FOURTH-ORDER RUNGE-KUTTA METHOD TO INTEGRATE   00000020
```

```
C          ORDINARY DIFFERENTIAL EQUATIONS SUPPLIED BY THE CALLING       00000030
C          PROGRAM. SINCE THESE EQUATIONS MUST BE REPEATEDLY QUOTE       00000040
C          CALLED UNQUOTE BY THIS PROGRAM, A COMPUTED GO TO IS HERE      00000050
C          USED TO ENSURE RETURN TO THE CORRECT PART OF THIS SUBROUTINE. 00000060
*                                                                        *0-   70
C         COMPLETED NOVEMBER 1963                                        00000080
C          REVISED JUNE 1964 AND JUNE 1965                               00000090
      DIMENSION X(30), DX(30), C(15), XC(30), ITITLE(12), JTITLE(10),   00000100
     1          KTITLE(10), X1(900), X2(900), X3(900), X4(900),         00000110
     2          Y1(900), Y2(900), Y3(900), Y4(900), IP(10), IG(10),     00000120
     3          PR(10), GR(10) ,TX(6), TY(6)                            00000130
      INDIC = C(10)                                                     00000140
      GO TO (1, 2000, 50, 58, 88, 88),INDIC                             00000150
*                                                                       0000 160
C          READ DATA AND PRINT RECORD.                                   00000170
*                                                                       0000 180
    1 READ 100, (ITITLE(I), I=1,6 )                                     00000190
      READ 101,NR                                                       00000200
      READ 102, NN                                                      00000210
      NRC = 0                                                           0000 220
      IF(NN- 30)1000,1000,2                                             00000230
    2 PRINT 200                                                         00000240
      STOP                                                              0000 250
 1000 NRC = NRC + 1                                                     00000260
      PRINT 201, (ITITLE(I), I=1,6)                                     00000270
      IF (NRC - 1)6,3,6                                                 00000280
    3 IF (NR - 1)4,5,4                                                  00000290
    4 PRINT 202, NR                                                     00000300
      GO TO 6                                                           00000310
    5 PRINT 203                                                         00000320
      GO TO 7                                                           00000330
    6 PRINT 204, NRC                                                    00000340
    7 PRINT 205, NN                                                     00000350
  100 FORMAT (10A8)                                                     00000360
  101 FORMAT (I1)                                                       00000370
  102 FORMAT (I2)                                                       00000380
```

```
200 FORMAT (////,48H ERROR IN ORDER OF EQUATION. MUST NOT EXCEED 30. )00000390
201 FORMAT (1H1,/////,36X,6A8)                                        00000400
202 FORMAT (/,37X,I1,20H RUNS ARE CALLED FOR )                        00000410
203 FORMAT (/,37X,21HONE RUN IS CALLED FOR ,///,18H INPUT DATA RECORD)00000420
204 FORMAT (///,34H INPUT DATA RECORD FOR RUN NUMBER  ,I1)            00000430
205 FORMAT (//,22H ORDER OF EQUATIONS = ,I2)                          00000440
    READ 103, TI, DT, TF1, DT2, TF2, DT3, TF3                        00000450
103 FORMAT (8F10.4)                                                  00000460
    IF(DT2)9,8,9                                                     00000470
  8 TF = TF1                                                         00000480
    PRINT 206, TI, TF                                                00000490
    PRINT 207,DT                                                     00000500
206 FORMAT (22H INITIAL TIME        = ,E10.4,/                       00000510
   1        22H FINAL TIME          = ,E10.4)                        00000520
207 FORMAT (22H STEP SIZE           = ,E10.4)                        00000530
    GO TO 12                                                         00000540
  9 IF(DT3)11,10,11                                                  00000550
 10 TF = TF2                                                         00000560
    PRINT 206, TI, TF                                                00000570
    PRINT 208, DT, TI, TF1, DT2, TF1, TF                             00000580
208 FORMAT (22H STEP SIZE           = ,E10.4,13H BETWEEN T = ,E10.4,  00000590
   1         9H AND T = ,E10.4)                                      00000600
    GO TO 12                                                         00000610
 11 TF = TF3                                                         00000620
    PRINT 206, TI, TF                                                00000630
    PRINT 208, DT, TI, TF1, DT2, TF1, TF2, DT3, TF2, TF              00000640
 12 READ 103, (C(I), I=1,8)                                          00000650
    READ 103, (X(I), I=1,NN)                                         00000660
    J = 0                                                            000 670
    DO 14 I=1,8                                                      00000680
    IF(C(I))13,14,13                                                 00000690
 13 J = J + 1                                                        00000700
 14 CONTINUE                                                         00000710
    K = 0                                                            0000 720
    DO 16 I=1,NN                                                     00000730
    IF(X(I))15,16,15                                                 00000740
```

```
   15 K = K + 1                                                          00000750
   16 CONTINUE                                                           00000760
      IF(J - 1)17,18,19                                                  00000770
   17 PRINT 209                                                          00000780
      GO TO 423                                                          00000790
   18 PRINT 210                                                          00000800
      GO TO 420                                                          00000810
   19 PRINT 211                                                          00000820
  420 DO 422 I=1,8                                                       00000830
      IF(C(I))421,422,421                                                00000840
  421 PRINT 212, I, C(I)                                                 00000850
  422 CONTINUE                                                           00000860
  209 FORMAT (/,34H ALL THE CONSTANTS, C(I), ARE ZERO )                  00000870
  210 FORMAT (/,30H THE ONLY NON-ZERO CONSTANT IS )                      00000880
  211 FORMAT (/,35H THE NON-ZERO CONSTANTS, C(I), ARE )                  00000890
  212 FORMAT (14X,2HC(,I2,4H) = ,E10.4)                                  00000900
  423 IF(K - 1)424,425,426                                               00000910
  424 PRINT 1209                                                         00000920
      GO TO 20                                                           00000930
  425 PRINT 1210                                                         00000940
      GO TO 427                                                          00000950
  426 PRINT 1211                                                         00000960
  427 DO 429 I=1,NN                                                      00000970
      IF(X(I))428,429,428                                                00000980
  428 PRINT 1212, I, X(I)                                                00000990
  429 CONTINUE                                                           00001000
 1209 FORMAT (/,36H ALL THE INITIAL CONDITIONS ARE ZERO )                00001010
 1210 FORMAT (/,39H THE ONLY NON-ZERO INITIAL CONDITION IS )             00001020
 1211 FORMAT (/,36H THE NON-ZERO INITIAL CONDITIONS ARE )                00001030
 1212 FORMAT (14X,2HX(,I2,4H) = ,E10.4)                                  00001040
   20 READ 104, (JTITLE(I), IP(I), I = 1,8)                              00001050
  104 FORMAT(8(A8,I2))                                                   00001060
*                                                                        00001070
C     CHECK FOR THE NUMBER OF COLUMNS CALLED FOR BY LOCATING FIRST       00001080
C     BLANK COLUMN HEADING                                               00001090
*                                                                        00001100
```

```
      IBLANK = 8H                                                       00001110
      DO 21 J=1,8                                                       00001120
      IF(JTITLE(J) - IBLANK)21,22,21                                    00001130
   21 CONTINUE                                                          00001140
      J = 9                                                             00001150
   22 JJ = J - 1                                                        00001160
*                                                                       00001170
C     JJ IS NOW THE NUMBER OF COLUMNS. REPEAT WITH THE GRAPHS.          00001180
*                                                                       00001190
      READ 105, (KTITLE(I), KTITLE(I+1), IG(I), IG(I+1), I=1,7,2)       00001200
  105 FORMAT (4(2A8,2I2))                                               00001210
      DO 24 K=1,7,2                                                     00001220
      IF(KTITLE(K) - IBLANK)24,23,24                                    00001230
   23 IF(KTITLE(K+1) - IBLANK)24,25,24                                  00001240
   24 CONTINUE                                                          00001250
      K = 8                                                             00001260
   25 KK = K/2                                                          00001270
      KKK = KK*2                                                        00001280
      MULTIP = 0                                                        00001290
      IF(KK -1)306,300,306                                              00001300
  300 IF(IG(3) + IG(4))301,306,301                                      00001310
  301 IF(IG(5) + IG(6))303,302,303                                      00001320
  302 MULTIP = 2                                                        00001330
      KKK = 4                                                           00001340
      GO TO 306                                                         00001350
  303 IF(IG(7) + IG(8))305,304,305                                      00001360
  304 MULTIP = 3                                                        00001370
      KKK = 6                                                           00001380
      GO TO 306                                                         00001390
  305 MULTIP = 4                                                        00001400
      KKK = 8                                                           00001410
*                                                                       00001420
C     IF MULTIP = 0, KK IS THE NUMBER OF SINGLE CURVE GRAPHS. OTHERWISE 00001430
C     MULTIP IS THE NUMBER OF CURVES ON A SINGLE GRAPH.                 00001440
*                                                                       00001450
  306 IF(JJ)26,27,26                                                    00001460
```

```
   26 PRINT 214, (JTITLE(I), IP(I), I=1,JJ)                              00001470
  214 FORMAT (///,56H THE COLUMN HEADINGS AND THE CORRESPONDING VARIABLE00001480
     1S ARE ,//,(10X,A8,4X,2HX(,I2,1H)))                                00001490
      GO TO 28                                                          00001500
   27 PRINT 215                                                         00001510
  215 FORMAT (///,25H NO PRINTOUT IS REQUIRED  )                        00001520
   28 IF(KK)29,308,29                                                   00001530
   29 IF(MULTIP)309,30,309                                              00001540
   30 IF(KK - 1)307,1306,307                                            00001550
 1306 PRINT 216, KTITLE(1), KTITLE(2), IG(1), IG(2)                     00001560
  216 FORMAT (///,52H THE GRAPH TITLE AND THE CORRESPONDING VARIABLES AR00001570
     1E ,//,10X,2A8,4X,2HX(,I2,8H) VS. X(,I2,1H))                       00001580
      GO TO 31                                                          00001590
  307 PRINT 217, (KTITLE(I), KTITLE(I+1), IG(I), IG(I+1), I=1,KKK ,2)   00001600
  217 FORMAT (///,64H THE INDIVIDUAL GRAPH TITLES AND THE CORRESPONDING 00001610
     1VARIABLES ARE ,//,(10X,2A8,4X,2HX(,I2,8H) VS. X(,I2,1H)))         00001620
      GO TO 31                                                          00001630
  308 PRINT 1217                                                        00001640
 1217 FORMAT(///,24H NO GRAPHS ARE REQUIRED  )                          00001650
      GO TO 31                                                          00001660
  309 PRINT 1220                                                        00001670
 1220 FORMAT (///,52H THE GRAPH TITLE AND THE CORRESPONDING VARIABLES AR00001680
     1E ,/)                                                             00001690
      PRINT 1221, KTITLE(1), KTITLE(2), (IG(I), IG(I+1), I=1,KKK,2)     00001700
 1221 FORMAT (10X,2A8,4X,2HX(,I2,8H) VS. X(,I2,1H),/, (30X,2HX(,I2,     00001710
     1        8H) VS. X(,I2,1H)))                                       00001720
*                                                                       00001730
C     THIS ENDS THE BOOK-KEEPING. INITIALIZE BEFORE ENTERING MAIN LOOP. 00001740
*                                                                       00001750
   31 IPAGE = 0                                                         00001760
      T = TI                                                            00001770
      NOPTS = 0                                                         00001780
      NUMPTS = 0                                                        00001790
      ITITLE(8) = 8H                                                    00001800
      ITITLE(11)= 8H                                                    00001810
      ITITLE(12)= 8H                                                    00001820
```

```
      GO TO (32,33,34,35,36,37,38,39,40),NRC                                    00001830
   32 ITITLE(7) = 8H RUN 1                                                      00001840
      GO TO 41                                                                  00001850
   33 ITITLE(7) = 8H RUN 2                                                      00001860
      GO TO 41                                                                  00001870
   34 ITITLE(7) = 8H RUN 3                                                      00001880
      GO TO 41                                                                  00001890
   35 ITITLE(7) = 8H RUN 4                                                      00001900
      GO TO 41                                                                  00001910
   36 ITITLE(7) = 8H RUN 5                                                      00001920
      GO TO 41                                                                  00001930
   37 ITITLE(7) = 8H RUN 6                                                      00001940
      GO TO 41                                                                  00001950
   38 ITITLE(7) = 8H RUN 7                                                      00001960
      GO TO 41                                                                  00001970
   39 ITITLE(7) = 8H RUN 8                                                      00001980
      GO TO 41                                                                  00001990
   40 ITITLE(7) = 8H RUN 9                                                      00002000
   41 C(11) = 20.                                                               00002010
      C(12) = 5.                                                                00002020
      C(13) = DT                                                                00002030
      DO 42 I=1,NN                                                              00002040
   42 XC(I) = X(I)                                                              00002050
      TC = T                                                                    00002060
      C(10) = 2.                                                                00002070
      RETURN                                                                    00002080
 2000 IF(JJ)43,54,43                                                            00002090
   43 INCPR = C(11)                                                             00002100
      C(11) = 20.                                                               00002110
      IF(XMODF(NOPTS,50*INCPR))44,46,44                                         00002120
   44 IF(XMODF(NOPTS,10*INCPR))45,47,45                                         00002130
   45 IF(XMODF(NOPTS,   INCPR))54,48,54                                         00002140
   46 IPAGE = IPAGE + 1                                                         00002150
      IF(NR - 1)1046,1047,1046                                                  00002160
 1046 PRINT 218, (ITITLE(I), I=1,6), IPAGE, ITITLE(7), (JTITLE(I),I=1,8)00002170
      PRINT 219                                                                 00002180
```

```
      GO TO 47                                                          00002190
1047  PRINT 1218, (ITITLE(I), I=1,6), IPAGE, (JTITLE(I), I=1,8)         00002200
      PRINT 219                                                         00002210
   47 PRINT 219                                                         00002220
  218 FORMAT (1H1,///,20X,6A8,10X,5HPAGE ,I1,14H OF OUTPUT FOR,A8,/////,00002230
     1        11X,8(A8,5X))                                           00002240
1218  FORMAT (1H1,///,20X,6A8,30X,5HPAGE ,I1,/////,11X,8(A8,5X))       00002250
  219 FORMAT (1H  )                                                    00002260
   48 DO 49 I=1,NN                                                     00002270
   49 XC(I) = X(I)                                                     00002280
      TC = T                                                           00002290
      C(10) = 3.                                                       00002300
      RETURN                                                           00002310
   50 DO 53 I=1,JJ                                                     00002320
      IF(IP(I))52,51,52                                                00002330
   51 PR(I) = T                                                        00002340
      GO TO 53                                                         00002350
   52 IPI = IP(I)                                                      00002360
      PR(I) = XC(IPI)                                                  00002370
   53 CONTINUE                                                         00002380
      PRINT 220, (PR(I), I=1,JJ)                                       00002390
 220  FORMAT (7X, 8E13.5)                                              00002400
   54 IF(KK)55,62,55                                                   00002410
   55 INCGR = C(12)                                                    00002420
      C(12) = 5.                                                       00002430
      IF(XMODF(NOPTS, INCGR))62,56,62                                  00002440
   56 DO 57 I=1,NN                                                     00002450
   57 XC(I) = X(I)                                                     00002460
      TC = T                                                           00002470
      C(10) = 4.                                                       00002480
      RETURN                                                           00002490
   58 DO 61 I=1,KKK                                                    00002500
      IF(IG(I))60,59,60                                                00002510
   59 GR(I) = T                                                        00002520
      GO TO 61                                                         00002530
   60 IGI = IG(I)                                                      00002540
```

```
      GR(I) = XC(IGI)                                                    00002550
   61 CONTINUE                                                           00002560
      IF(KKK - 8)1611,1610,1610                                          00002570
 1611 KP1 = KKK + 1                                                      00002580
      DO 1612 I=KP1,8                                                    00002590
 1612 GR(I) = 0.                                                         00002600
 1610 NUMPTS = NUMPTS + 1                                                00002610
      Y1(NUMPTS) = GR(1)                                                 00002620
      X1(NUMPTS) = GR(2)                                                 00002630
      Y2(NUMPTS) = GR(3)                                                 00002640
      X2(NUMPTS) = GR(4)                                                 00002650
      Y3(NUMPTS) = GR(5)                                                 00002660
      X3(NUMPTS) = GR(6)                                                 00002670
      Y4(NUMPTS) = GR(7)                                                 00002680
      X4(NUMPTS) = GR(8)                                                 00002690
   62 NOPTS = NOPTS + 1                                                  00002700
      IF(NUMPTS - 900)64,63,64                                           00002710
   63 PRINT 221                                                          00002720
  221 FORMAT (//////,25H STOP AT 900 GRAPH POINTS    )                   00002730
      GO TO 91                                                           00002740
   64 IF(NOPTS - 4500)66,65,66                                           00002750
   65 PRINT 222                                                          00002760
  222 FORMAT (//////,31H STOP AT 4500 INTEGRATION STEPS  )               00002770
      GO TO 91                                                           00002780
   66 IF(IPAGE - 9)69,67,68                                              00002790
   67 IF(XMODF(NOPTS , 50*INCPR))69,68,69                                00002800
   68 PRINT 223                                                          00002810
  223 FORMAT (//////,27H STOP AT 9 PAGES OF OUTPUT   )                   00002820
      GO TO 91                                                           00002830
   69 DO 70 I=1,NN                                                       00002840
      IF(ABSF(X(I)) - 1.0E+12)70,70,71                                   00002850
   70 CONTINUE                                                           00002860
      GO TO 72                                                           00002870
   71 PRINT 224                                                          00002880
  224 FORMAT (//////,76H STOP WITH THE ABSOLUTE VALUE OF A DEPENDENT VAR00002890
     1IABLE GREATER THAN 1.0E+12.  ,/,57H INTEGRATION PROBABLY UNSTABLE.00002900
```

```
   2 TRY A SMALLER STEP SIZE. ,26HNO GRAPHS WILL BE PLOTTED.       )  00002910
     GO TO 330                                                        00002920
  72 DT = C(13)                                                       00002930
     IF(TI - TF)73,73,80                                              00002940
  73 IF(T - TF)75,74,74                                               00002950
  74 PRINT 225                                                        00002960
 225 FORMAT (//////,26H NORMAL STOP AT FINAL TIME    )               00002970
     GO TO 91                                                         00002980
  75 IF(T - TF1)76,77,77                                              00002990
  76 C(13) = DT                                                       00003000
     GO TO 87                                                         00003010
  77 IF(T - TF2)78,79,79                                              00003020
  78 C(13) = DT2                                                      00003030
     GO TO 87                                                         00003040
  79 C(13) = DT3                                                      00003050
     GO TO 87                                                         00003060
  80 IF(TF - T)82,74,74                                               00003070
  82 IF(TF1 - T)76,84,84                                              00003080
  84 IF(TF2 - T)78,79,79                                              00003090
  87 C(10) = 5.                                                       00003100
  88 CALL RKUTTA2(NN, T, X, DT, C, TC, XC, DX)                        00003110
     IF(C(10) - 6.)90,89,90                                           00003120
  89 RETURN                                                           00003130
  90 T = T + DT                                                       00003140
     GO TO 2000                                                       00003150
  91 IF(KK)92,330,92                                                  00003160
  92 IF(MULTIP)97,93,97                                               00003170
  93 LABEL = 4H                                                       00003180
     ITITLE(9) = KTITLE(1)                                            00003190
     ITITLE(10)= KTITLE(2)                                            00003200
     CALL DRAW (NUMPTS,Y1,X1,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,00003211
    1           LAST)                                                 00003212
     IF(KK - 1)94,330,94                                              00003220
  94 ITITLE(9) = KTITLE(3)                                            00003230
     ITITLE(10)= KTITLE(4)                                            00003240
     CALL DRAW (NUMPTS,Y2,X2,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,00003251
```

```
     1           LAST)                                                    00003252
      IF(KK - 2)95,330,95                                               00003260
   95 ITITLE(9) = KTITLE(5)                                             00003270
      ITITLE(10)= KTITLE(6)                                             00003280
      CALL DRAW (NUMPTS,Y3,X3,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,00003291
     1           LAST)                                                  00003292
      IF(KK - 3)96,330,96                                               00003300
   96 ITITLE(9) = KTITLE(7)                                             00003310
      ITITLE(10)= KTITLE(8)                                             00003320
      CALL DRAW (NUMPTS,Y4,X4,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,00003331
     1           LAST)                                                  00003332
      GO TO 330                                                         00003340
*                                                                       00003350
C     NOW PLOT DUMMY CURVE ALONG AXES TO SET SCALES.                    00003360
*                                                                       00003370
   97 BIGX = 0.                                                         00003380
      BIGY = 0.                                                         00003390
      SMLX = 0.                                                         00003400
      SMLY = 0.                                                         00003410
      DO 1970 I=1,NUMPTS                                                00003420
      XMAX = MAX1F ( X1(I), X2(I), X3(I), X4(I))                        00003430
      YMAX = MAX1F ( Y1(I), Y2(I), Y3(I), Y4(I))                        00003440
      XMIN = MIN1F (X1(I), X2(I), X3(I), X4(I))                         00003450
      YMIN = MIN1F( Y1(I), Y2(I), Y3(I), Y4(I))                         00003460
      IF (BIGX - XMAX) 1971,1972,1972                                   00003470
 1971 BIGX = XMAX                                                       00003480
 1972 IF (BIGY-YMAX)1973,1974,1974                                      00003490
 1973 BIGY = YMAX                                                       00003500
 1974 IF (SMLX - XMIN) 1976,1976,1975                                   00003510
 1975 SMLX = XMIN                                                       00003520
 1976 IF (SMLY - YMIN)1970,1970,1977                                    00003530
 1977 SMLY = YMIN                                                       00003540
 1970 CONTINUE                                                          00003550
      TX(1) = 0.                                                        00003560
      TX(2) = 0.                                                        00003570
      TX(3) = 0.                                                        00003580
```

```
      TX(4) = SMLX                                                          00003590
      TX(5) = BIGX                                                          00003600
      TY(1) = BIGY                                                          00003610
      TY(2) = SMLY                                                          00003620
      TY(3) = 0.                                                            00003630
      TY(4) = 0.                                                            00003640
      TY(5) = 0.                                                            00003650
      LABEL = 4H                                                            00003660
      ITITLE(9) = KTITLE(1)                                                 00003670
      ITITLE(10)= KTITLE(2)                                                 00003680
      CALL DRAW (5,TX,TY,1,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,1,LAST)
      MODCURV = 2                                                           00003700
      LABEL = 4H 1                                                          00003710
      CALL DRAW (NUMPTS,X1,Y1,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)                                                    00003730
      IF(MULTIP - 2)98,98,99                                                00003740
   98 MODCURV = 3                                                           00003750
      GO TO 325                                                             00003760
   99 MODCURV = 2                                                           00003770
  325 LABEL = 4H 2                                                          00003780
      CALL DRAW (NUMPTS,X2,Y2,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)                                                    00003800
      IF(MULTIP - 3)330,326,327                                             00003810
  326 MODCURV = 3                                                           00003820
      GO TO 328                                                             00003830
  327 MODCURV = 2                                                           00003840
  328 LABEL = 4H 3                                                          00003850
      CALL DRAW (NUMPTS,X3,Y3,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)                                                    00003870
      IF(MULTIP - 4)330,329,329                                             00003880
  329 MODCURV = 3                                                           00003890
      LABEL = 4H 4                                                          00003900
      CALL DRAW (NUMPTS,X4,Y4,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)                                                    00003920
  330 IF(NRC - NR)1000,331,1000                                             00003930
  331 IF(NR - 1)333,332,333                                                 00003940
```

```
332 PRINT 226                                                                    00003950
    STOP                                                                        00003960
333 PRINT 227, NR                                                               00003970
    STOP                                                                        00003980
226 FORMAT(//,43H THE ONE RUN CALLED FOR HAS BEEN COMPLETED. ,//)               00003990
227 FORMAT(//,5H THE ,I1,37H RUNS CALLED FOR HAVE BEEN COMPLETED.,//)           00004000
    END                                                                         00004010
    SUBROUTINE RKUTTA2(NN, T, X, DT, C, TC, XC, DX)                             00004020
    DIMENSION X(30), C(15), XC(30), DX(30), CT(4), AK(4,30)                     00004030
    INDIC = C(10) - 4.0                                                         00004040
    GO TO (1, 3),INDIC                                                          00004050
  1 CT(1) = 0.0                                                                 00004060
    CT(2) = 0.5                                                                 00004070
    CT(3) = 0.5                                                                 00004080
    CT(4) = 1.0                                                                 00004090
    DO 4 II=1,4                                                                 00004100
    TC = T + CT(II)*DT                                                          00004110
    DO 2 J=1,NN                                                                 00004120
  2 XC(J) = X(J) + CT(II)*AK(II-1, J)                                           00004130
    C(10) = 6.0                                                                 00004140
    RETURN                                                                      00004150
  3 DO 4 J=1,NN                                                                 00004160
  4 AK(II, J) = DT*DX(J)                                                        00004170
    DO 5 J=1,NN                                                                 00004180
  5 X(J) =X(J) + (AK(1,J) + 2.*AK(2,J) + 2.*AK(3,J) + AK(4,J))/6.0              00004190
    C(10) = 7.0                                                                 00004200
    RETURN                                                                      00004210
    END                                                                         00004220
    END
```

Typical Input Data

Note: The data cards are in the same order as their explanation

```
 GAGLIANO, ROSS A.  TRAJECTORIES
1
 2
    .00   0.005       0.06       0.0005    0.1600     0.005      0.5000
    300.0  1.20
     .00  1.000
Z DIST  00RADIUS  01SLOPE   02
    45.00        0100
```

Typical Output Data

GAGLIANO, ROSS A. TRAJECTORIES

Z DIST	RADIUS	SLOPE
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]

NORMAL [illegible]

GRAPH TITLED . . [illegible], ROSS A. TRAJECTORIES
[illegible]

THE ONE RUN CALLED FOR [illegible] COMPLETED.

STOP
TIME, 2 MINUTES AND [illegible] SECONDS

APPENDIX 7

GRAPHS OF VARIOUS TRAJECTORIES

This appendix contains these four figures which show trajectories as produced by PROGRAM ORBITS.

Figure 3. The Standard Trajectory

Figure 4. Variation in Energy

Figure 5. Variation in Magnetic Field

Figure 6. Variation in Initial(scattering) Angle

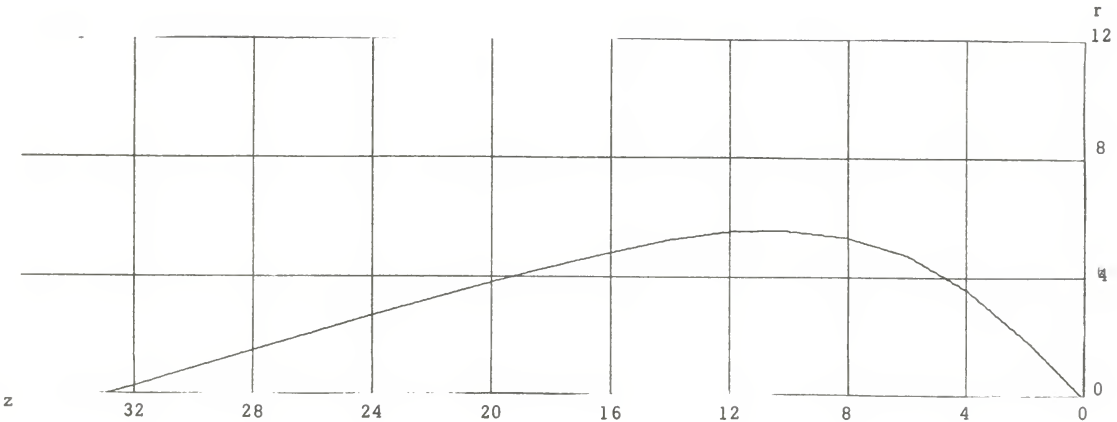


Fig. 3. The Standard Trajectory
The energy E_o = 300 eV, and the magnetization current is 12 amps. The scattering (initial) angle is 45°.

NOTE: From the origin in the lower right hand corner, the radial distance (r) is plotted versus the axial distance (z), and both are in centimeters. Further, z is positive to the left.

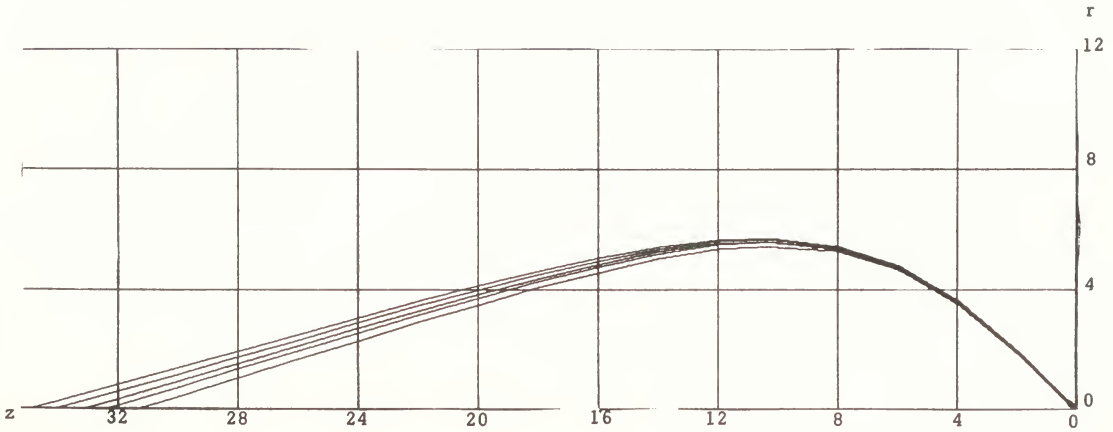


Fig. 4. Trajectories showing variation in energy

The field and initial angle were held constant, magnetization current of 12 amps and $\Theta = 45^{\circ}$.

The energy E_o was varied as follows: 300 ± 5 eV and 300 ± 10 eV.

The above curves range from 290 eV (the lowest curve) to 310 eV (the highest).

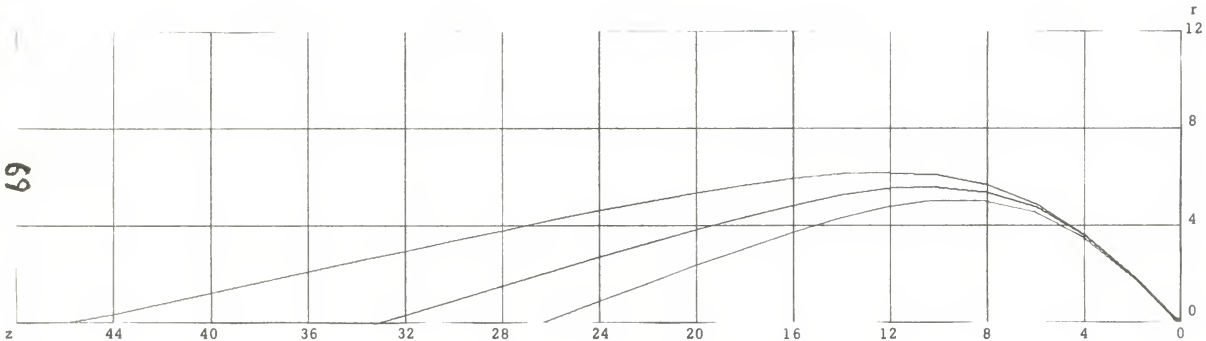


Fig. 5. Trajectories showing variation in magnetic field
The magnetizing current has values of 11, 12 and 13 amps.
E_o = 300 eV and $\Theta = 45^o$, and both were held constant.

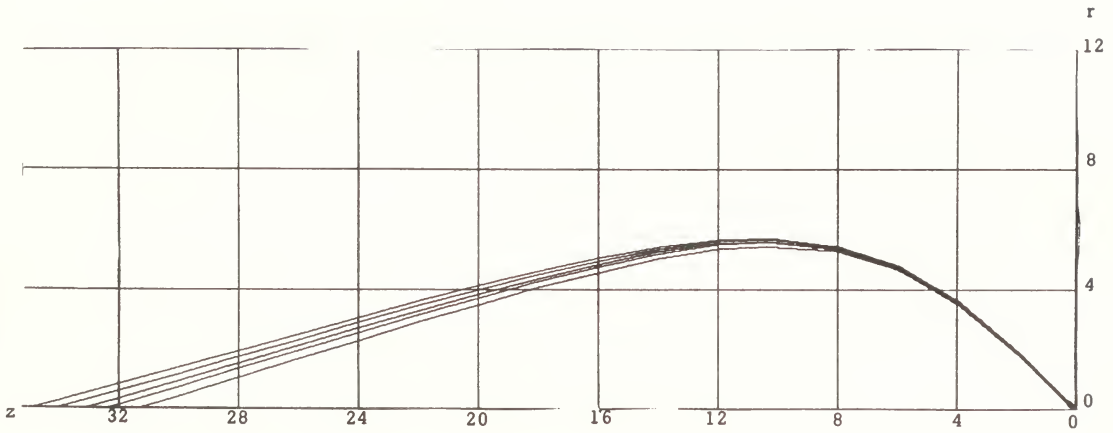


Fig. 4. Trajectories showing variation in energy

The field and initial angle were held constant, magnetization current of 12 amps and $\Theta = 45^{\circ}$.

The energy E_o was varied as follows: 300 ± 5 eV and 300 ± 10 eV.

The above curves range from 290 eV (the lowest curve) to 310 eV (the highest).

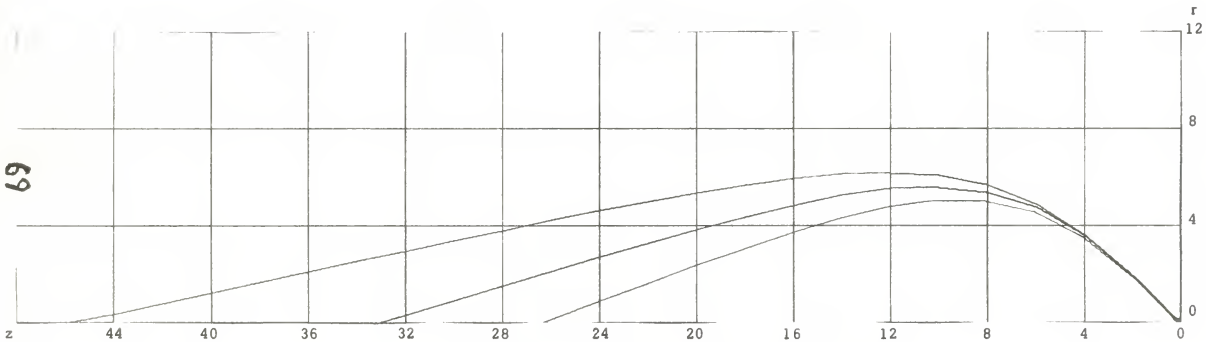


Fig. 5. Trajectories showing variation in magnetic field
The magnetizing current has values of 11, 12 and 13 amps.
E_o = 300 eV and $\Theta = 45^o$, and both were held constant.

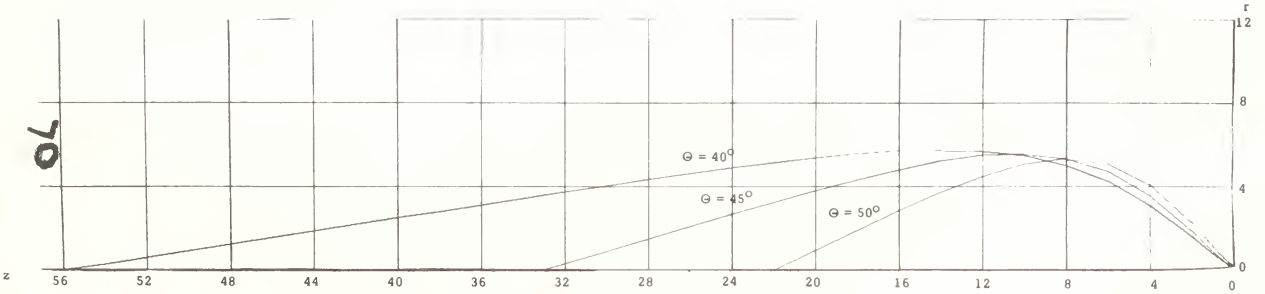


Fig. 6. Trajectories showing variation in initial angle, where Θ is varied as shown above. E_o = 300 eV and the magnetization current = 12 amps.

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13. ABSTRACT

This theoretical study of the trajectories of charged particles supplements an experimental project of molecular-ionic rearrangements using the magnetic focusing properties of a beta-ray spectrometer. The experimentally measured magnetic field was analytically represented by a twelfth-order polynomial. This field is axially symmetric, but non-homogeneous otherwise. The particular particle of concern was the hydrogen ion, H_2^+. The trajectory of this particle was computed from a second-order differential equation, assuming values for the kinetic energy and initial angle of the particle, and the magnetizing current. The solution was obtained by numerical integration using a CDC 1604 digital computer. The distinctive feature of these calculations, in contrast to those used normally for a beta-ray spectrometer, is the large scattering (initial) angle, about 45°.

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14. KEY WORDS	LINK A		LINK B		LINK C	
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